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DATA EVALUATION PROBLEMS IN REACTOR PHYSICS
THEORY OF PROGRAM RFIT

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ABSTRACT

The paper gives the theoretical background of program RFIT. This is a general purpose data evaluation program which may be adapted to a wide variety measurements. The problems are formulated in terms of experiments in reactor physics but the applicability of the results and of program RFIT is not restricted to this particular field.

After a short review of the main well known theorems of mathematical statistics needed in the paper, the statistical properties of the parameter estimates are treated for the maximum likelihood and the least squares methods A good deal of the paper is devoted to methods of verifying the goodness of fit i.e. the correctness of both the measured data and the theory underlying the evaluation. To this end, several statistical tests are suggested. Finally, some special problems are treated such as the corrections to be applied to the primarily measured data and the treatment of repeated measurements.

АННОТАЦИЯ

В отчете описываются теоретические основы программы RFIT. Это общая программа для обработки данных, полученных из разновидных экспериментов. Затронутые проблемы сформулированы по реакторной физике, а возможности использования результатов отчета и самой программы не огроничиваются этой специальной областью.

После обобщения общеизвестных теорем математической статистики, в отчете описаны статистические характеристики оценок по методам максимального правдоподобия и наименьших квадратов. Большая часть отчета посвящена таким проблемам, как проверка правильности экспериментальных данных и теории на которой обоснована обработка. В этих целях предложены различные методы проверки гипотез. Потом анализировалы некоторые специальные проблемы, например, вопрос поправок или обработка повторных измерений.

KIVONAT

A dolgozat leirja az RFIT program elméleti alapjait. Ez egy általános célu adatkezelő program, amelyet a mérések széles körére alkalmazni lehet. A problémákat a reaktorfizika fogalmai alapján fogalmazzuk meg, de az eredmények és a program alkalmazhatósága nem szoritkozik erre a speciális területre.

A matematikai statisztika általánosan ismert fő tételeinek a rövid áttekintése után tárgyaljuk a maximális valószinüség és a legkisebb négyzetek módszerének a statisztikai tulajdonságait. A dolgozat jelentős része foglalkozik az illesztés jóságának a vizsgálatára szolgáló módszerekkel, tehát azzal, hogyan lehet ellenőrizni egyrészt a mérési adatoknak, másrészt a kiértékelés alapjául szolgáló elméletnek a korrektségét. Ebből a célból néhány statisztikai tesztet javasolunk. Végül néhány speciális kérdéssel foglalkozunk, mint például a nyers mérési adatokhoz alkalmazandó korrekciók kérdése vagy ismételt mérések kezelése.

CONTENTS

NOMENCLATURE

$\underline{y}$	vector of the measured values with components $y_i (i=1,2,...,n)$
$\underline{x}$	vector of the values of the independent variable/s/ with components $x_i (i=1,2,..,n)$
$\underline{a}$	vector of the unknown parameters $a_k (k=1,2,...,m)$
n	number of measured points
m	number of unknown parameters
$f(x,\underline{a})$	fitting function
w_i	weight of point i
Q	the sum of square to be minimized in the least squares method
$L(\underline{x},\underline{y},\underline{a})$ $L(x_i,y_i,\underline{a})$	likelihood function
σ^2	a factor of proportionality: σ^2/w_i is the variance of point i
$P\{\ \}$	probability of the event in the brackets
$<\xi>$	expectation value of random variable ξ
$\tilde{a}_k$	estimate of a_k
$\tilde{y}_i$	estimate of $<y_i>$
y_i^*	unbiased estimate of $<y_i>$
σ_i^*	standard deviation of $\tilde{y}_i$ and y_i^*
a_k^*	estimate of a_k corrected for the bias
δa_k	bias of estimate $\tilde{a}_k$ $(= <\tilde{a}_k> - a_k)$
δy_i	bias of $\tilde{y}_i$ $(= <\tilde{y}_i> - f(x_i,\underline{a}))$
Δa_k	a random variable equal to $\tilde{a}_k - <\tilde{a}_k>$
$\Delta\tilde{a}_k$	standard deviation of estimate a_k $(= \sqrt{<(\Delta a_k)^2>})$
Δy_i	a random variable equal to $y_i - <y_i>$
$N(a,\sigma)$	set of Gaussian random variables with mean a and standard deviation σ
$\{\underline{\underline{A}}\}_{kk'}$	element (k,k') of matrix $\underline{\underline{A}}$
ξ	a Gaussian random variable, most frequently $N(0,1)$
t	Student fraction /except Chapter I. and section V.1./
γ	quantile of the Student distribution
γ_f	quantile of the Fisher distribution
γ_φ	quantile of the φ-distribution /see Appendix 2/

NOMENCLATURE (CONTINUED)

γ_{χ^2}	quantile of the χ^2 - distribution
ε	confidence probability
I_ℓ	set of subscripts i taken into account in point drop step ℓ
L	maximum number of steps
$\underline{a}_\ell$	parameter estimate in step ℓ
Q_ℓ	the minimum value of Q in step ℓ
n_ℓ	number of points in step ℓ
ν_i	dead time correction factor for point i
μ_{di}	decay correction factor for point i
α_i	additive correction for point i

INTRODUCTION

In a typical reactor physics experiment, not that quantity is measured directly which is actually needed. This has led to complicated data reduction and evaluation techniques. Their basis is commonly the method of least squares. The method itself is treated in a large number of textbooks /e.g. refs. [1],[2], or [3]/. Consequently, very little new can be said about it now. There have been, however, some important changes in reactor physics experimentation which make a reconsideration of the data evaluation problems necessary. These new aspects may be summarized as follows:

- Measurements are carried out in international cooperations. This requires that the standards of data evaluation must be agreed upon. Otherwise, it cannot be assured that the users of the evaluated results understand them in the same sense as the evaluator did.

- Rough experimental data appear in tremendous quantities. We went over to a mass production of experimental data. Data evaluation techniques should minimize the effort required from the experimentators. Man should do only what machine is not able to do: he has to plan the experiment, interprete the results, and judge their value. The computer has to do everything else, especially a detailed analysis of the data on which judgement and interpretation can firmly be based.

- Evaluated results will be used for checking calculations, testing hypotheses and they will induce changes somewhere else, e.g. in nuclear data libraries or in calculational models. It is important that evaluated results represent exactly the information content of the rough data. Not more, not less but that in an unbiased way.

- There are some problems specific to reactor physics experiments the statistical theory of which is not sufficiently well elaborated.

The purpose of the present paper is to describe the theoretical foundations of program RFIT. This is a general fitting program which takes these points of view into account. Before starting the detailed treatment of the subject, some general remarks are made.

Data evaluation is often called data reduction. This expression hits the nail on the head. Simply due to their volume, rough experimental data are difficult to survey and one has to reorganize and reduce them to a set of quantities of smaller extent in order to get the information one is interested in. Such a reduction entails an unavoidable loss of information. If, after data reduction, one is interested in something else, this is hardly to be found in the reduced set of data.One has rather to return to the original rough data and reevaluate them from the new point of view. That is why RFIT supposes the user to input rough experimental data to it.

Most fitting programs carry out the data reduction, print out the results and estimate the errors. When, however, something goes wrong with the data reduction or the user of the program wishes to make some decision on the basis of the program output, he is left to himself. The program does not come to his help although this would not require too much additional computation. As it will be seen later in this paper, the theory of a mathematical statistics method might be very sophisticated but the final formulae are relatively simple so that they may be incorporated in a fitting program with not too much effort.A great deal of this paper is devoted to the theoretical background of such additional services of program RFIT. Of course, they are powerful tools if they are well understood by the program user but they can be completely misleading if the conditions of their applicability are not met.

Program RFIT is the result of a continuous development /which will probably never stop/. All the problems solved by it arose from the practice of current reactor physics experiments. The methods described in this paper evolved in the course of a large number of discussions with potential users of the program. The author is deeply indepted to all of them for these stimulating discussions without which RFIT could not have become what it is now. Their list would be too long so that none of them is mentioned here by name.

Chapter I and part of chapter II are the summary of those general and well-known results of mathematical statistics which were used in writing the program.These chapters are therefore concise and details are given only in order to facilitate the understanding for those readers who are not familiar with mathematical statistics. Chapters III and IV give the theoretical fundamentals of the statistical tests performed by RFIT. Here again, the reader is not supposed to be acquainted with statistical tests. Chapter V treats some important special problems such as corrections, handling of repetitive measurements.

The paper contains numerical examples as illustration. They are not based on real measurements but on measurements simulated by a random number

generator. Such "sterile" cases were preferred to real ones because it is a priori known which result the evaluation ought to give. We shall have then the opportunity to check the applicability of our methods. The cases studied are listed in Appendix 10.

CHAPTER I.

ESTIMATION OF PARAMETERS

The estimation of unknown parameters is one of the basic problems of mathematical statistics. We have no place here even to sketch the relevant theory. The reader is referred to the literature. The book of Jánossy [1] gives a detailed treatment of the maximum likelihood method while Linnik [2] and Vander Waerden [3] treat the least squares method in full detail. These monographs give also further references on the topic. For those readers who are not familiar with mathematical statistics and who do not wish to look up things in the textbooks, we give the basic definitions and cite those theorems which are closely related to our subject. The present chapter and part of chapter II. will be devoted to the summary of these rather elementary facts. When possible, the statements will be proved here. The paper will refer for proofs to the literature only if they are too complicated.

I.1 Definitions

Suppose that the quantities y and x are measured and they are known to satisfy the equation

$$y = f(x,\underline{a}) \qquad /I.1.1/$$

where $\underline{a}$ is the vector of m unknonwn parameters: $a_1, a_2, \ldots, a_m$. The purpose of the measurement is just the determination of $\underline{a}$. The measurement is repeated n times resulting in the pairs of values x_i, y_i $(i=1,2,\ldots,n)$. Later in this paper, pairs (x_i,y_i) will be referred to as points of measurement. Generally, both x_i and y_i are random variables. For the moment, we assume that only y_i is random while x_i is exactly known. Most fitting programs are formulated under this condition but, as it will be shown in section I.2.2, this is not at all essential. It is added that x_i need not be a single variable but it may be a global notation for several ones.

As y_i is random, y_i and x_i do not satisfy eq. /I.1.1/ exactly. It is true only for the expectation values:

$$\langle y_i \rangle = f(x_i, \underline{a}) \ . \qquad /I.1.2/$$

This equation is the mathematical expression of the following two important conditions:

- the measurement of y_i is free from systematic errors and
- the choice of function $f(x,\underline{a})$ is physically proper.

These two conditions are not independent from each other because the improper choice of function $f(x,\underline{a})$ can be interpreted also as a systematic error.

For the estimation of the unknown parameters, many procedures are conceivable. Mathematically, estimation means that parameters a_k are expressed as functions of the measured quantities:

$$\tilde{a}_k = t_k(\underline{x},\underline{y}) \qquad /I.1.3/$$

$$(k = 1, 2, \ldots, m)$$

where $\underline{x}$ and $\underline{y}$ are vectors having for components $x_1, x_2, \ldots, x_n$ and $y_1, y_2, \ldots, y_n$, respectively. Estimates $\tilde{a}_k$ are random variables being functions of such ones. Their statistical properties are determined by the statistical behaviour of $\underline{y}$. We introduce, therefore, the <u>likelihood function</u> $L(\underline{x},\underline{y},\underline{a})$ which is defined as the probability density of $\underline{y}$. Usually, it may be supposed that different measurements are independent of each other, i.e. we suppose that

$$L(\underline{x},\underline{y},\underline{a}) = \prod_{i=1}^{n} L(x_i, y_i, \underline{a}) \ . \qquad /I.1.4/$$

/We hope that it won't lead to confusion that we use the same symbol L on both sides./ For example, if the measurement consists in counting, the Poissonian distribution applies:

$$L(x_i, y_i, \underline{a}) = e^{-f(x_i,\underline{a})} \frac{[f(x_i,\underline{a})]^{y_i}}{y_i!} \ . \qquad /I.1.5/$$

Using the likelihood function, the basic statistical properties of the estimates /I.1.3/ may easily be defined, e.g. expectation:

$$\langle \tilde{a}_k \rangle = \int t_k(\underline{x},\underline{y})\ L(\underline{x},\underline{y},\underline{a})\ d\underline{y} \qquad /I.1.6a/$$

and variance

$$\langle (\Delta a_k)^2 \rangle = \int \left[t_k(\underline{x},\underline{y}) - \langle \tilde{a}_k \rangle \right]^2 L(\underline{x},\underline{y},\underline{a})\ d\underline{y} \ . \qquad /I.1.6b/$$

From a satisfactory estimate, the following are required.

a/ It should be unbiased, i.e. the condition

$$\delta a_k = \langle \tilde{a}_k \rangle - a_k = 0 \qquad /I.1.7/$$

should be fulfilled for all k. If δa_k is not zero, it is called the bias of the estimate and may be considered as the systematic error of the estimation. This is to be distinguished from the systematic error of the measurement or the systematic error brought about by an improper choice of the function $f(x,\underline{a})$. Of course, if the latter types of systematic errors occur, the estimate will be surely biased but it should also be borne in mind that the estimation procedure itself can lead to some bias, too.

b/ One wants to have as small a variance as possible. There is now a theorem called the Cramér-Rao unequality /see e.g. [2]/ which says that there exists a minimum variance bound to all estimates. This bound depends only on the likelihood function. In a sense, it expresses the information content of the given measurement. We are naturally interested in extracting all this information i.e. we want $\langle (\Delta a_k)^2 \rangle$ to reach this minimum variance. Such an estimate is called efficient.

c/ Finally, there is an entirely practical requirement. The estimation should be realized by the available computational means in a reasonably short time.

Before going further, we remark that these requirements are practically never met in reactor physics. The point is that, in view of requirement c/, one is forced to choose simplified functions $f(x,\underline{a})$ which are not valid for the whole set of values x_i. One always has to reject some of them in order to meet requirement a/. Therefore, data evaluation in reactor physics means not only parameter estimation but also verification of the propriety of function $f(x,\underline{a})$. In practice, the set of measured points is reduced until the verification says that $f(x,\underline{a})$ is proper for some reduced set /see Chapter IV/. Quite naturally, it is always somewhat ambiguous when to stop such a reduction procedure. Thus some bias can not be surely avoided and the minimum variance bound will be floating. A considerable part of this paper will be devoted to the study of these problems but, for the time being, we have to assume that requirement a/ is met i.e. eq. /I.1.7/ holds.

It has been proved [1], [2] that it is the maximum likelihood method which gives the well behaved estimate what we need. According to this method, such values $\tilde{a}_k$ should be found which make likelihood function $L(\underline{x},\underline{y},\underline{a})$ maximal for the measured set $(\underline{x},\underline{y})$. Under some conditions [1] not cited here, it has some useful properties among which the following will be important for us:

- It is asymptotically efficient, i.e. $\langle(\Delta a_k)^2\rangle$ reaches the minimum variance bound when $n \to \infty$.
- The statistical behaviour of $\tilde{a}_k$ is asymptotically Gaussian.
- The estimate $\tilde{a}_k$ is asymptotically unbiased.

In practical cases, one has a finite number n of points. As to the first two properties, we will consider n to be sufficiently large. As to the third property, however, one must be careful. It is advisable to check in all practical cases whether the estimate is really unbiased. Very often, it is found not to be the case. Then the necessary correction should be applied.

The maximum likelihood method means that the set of equations

$$\frac{\partial \log L(\underline{x},\underline{y},\underline{a})}{\partial a_k} = 0 \qquad /I.1.8/$$

$$k = 1,2,\ldots,m$$

should be solved for a_k as unknowns while the measured values are substituted for $\underline{x}$ and $\underline{y}$. We shall call this the likelihood equation. When it is compared to eq. /I.1.3/, it is seen that estimate $t_k(\underline{x},\underline{y})$ is defined by eq. /I.1.8/ as an implicit function.

I.2 Important special cases. The method of least squares

The likelihood equation /I.1.8/ is too general. In practical cases, the form of the likelihood function has to be specialized. There are two important special cases in reactor physics experiments: Gaussian and Poissonian distributions. As it will be seen, the likelihood equation is reduced to a simpler form in these cases. This is the equation of the least squares method.

I.2.1 Gaussian distribution

The likelihood equation goes over into the well known least squares equation when the y_i are Gaussian random variables i.e. the likelihood function is given by

$$L(\underline{x},\underline{y},\underline{a}) = \frac{1}{(2\pi)^{n/2} \prod_{i=1}^{n} \sigma_i} \exp\{-\frac{1}{2} \sum_{i=1}^{n} \frac{1}{\sigma_i^2}[y_i - f(x_i,\underline{a})]^2\} \qquad /I.2.1/$$

where σ_i^2 is the variance of y_i:

$$\sigma_i^2 = \langle(\Delta y_i)^2\rangle \; . \qquad /I.2.2/$$

This function is at a maximum when

$$\sum_{i=1}^{n} \frac{1}{\sigma_i^2} \left[y_i - f(x_i, \underline{a})\right]^2 = \text{minimum}.$$

For convenience, we introduce weights w_i instead of σ_i^2 according to the formula

$$\sigma_i^2 = \frac{\sigma^2}{w_i} \qquad /I.2.3/$$

where σ^2 is some constant /arbitrary for the time being/. We have now the following recipe for the determination of estimates $\tilde{\underline{a}}$:

$$Q(\tilde{\underline{a}}) = \sum_{i=1}^{n} w_i \left[y_i - f(x_i, \tilde{\underline{a}})\right]^2 = \text{minimum} \qquad /I.2.4/$$

which is the <u>weighted least squares condition.</u>

The likelihood equation /I.1.8/ now has the form

$$\frac{\partial Q}{\partial a_k} = 0.$$

$$k = 1,2,\ldots,m$$

It will be useful in the following to introduce functions

$$G_k(\tilde{\underline{a}}) = -\frac{1}{2} \frac{\partial Q}{\partial a_k} = \sum_{i=1}^{n} w_i \left[y_i - f(x_i, \tilde{a})\right] \frac{\partial f(x_i, \tilde{\underline{a}})}{\partial a_k} \qquad /I.2.5/$$

$$k = 1,2,\ldots,m$$

and form vector function $\underline{G}(\tilde{\underline{a}})$ from them as components. Then the likelihood equation may be written as

$$\underline{G}\ (\tilde{\underline{a}}) = 0. \qquad /I.2.6/$$

This set of equations may be solved by iteration. The problems connected with it will be taken up in section I.3.

I.2.2 <u>The case when x_i is random</u>

Up to now, it was assumed that independent variable x_i is exactly known. This is acceptable e.g. when x_i is the time variable which can be measured rather accurately. When x_i is the position where a foil was irradi-

ated within the reactor, the uncertainty of its positioning is, however, hardly negligible. Later in this paper /see chapter V/, we shall see other reasons why we have to study how to account for the random character of x_i.

We distinguish two cases. As we shall see, they differ only principally but the corresponding estimation procedures are formally identical. In tne first case, only the nominal value x_{io} of x_i is known but it is unknown what the value of x_i was in the actual measurement. If, for example, x_i is the position of a fuel element in the reactor, only its nominal position in the lattice is known but it is generally not measured where an individual fuel element is displaced due to bending or for other reasons. This modifies the distribution of y_i. In the second case, we have only a measured value for x_i but its expectation x_{io} is unknown. Now the distribution of y_i depends on x_{io} through its expectation $f(x_{io},\underline{a})$ /see eq. /I.1.2//. Consequently, we have to estimate not only the unknown parameter vector $\underline{a}$ but also all x_{io}.

For the treatment of such cases, we need a distribution function for x_i. We assume that $x_i \in N(x_{io},\sigma_{xi})$ i.e. the probability density of x_i is written as

$$\varphi(x_i) = \frac{1}{\sigma_{x_i}\sqrt{2\pi}} \exp\{ - \frac{(x_i-x_{io})^2}{2\sigma_{x_i}^2} \}. \qquad /I.2.7/$$

The meaning of σ_{xi} is slightly different in the two cases: it is the standard deviation of the distribution of the possible x_i values in the first case, while it is the standard deviation of the measurement of x_i in the second case. There is also a difference as to what is known: x_{io} in the first, x_i in the second case.

As different measurements are statistically independent, it is sufficient to consider how the distribution of one of the y_i variables changes in the first case. Eq. /I.2.1/ gives in fact only the conditional probability density function of y_i as

$$L(y_i,\underline{a}|x_i) = \frac{1}{\sigma_{y_i}\sqrt{2\pi}} \exp\{ - \frac{[y_i-f(x_i,\underline{a})]^2}{2\sigma_{y_i}^2}\} .$$

Taking into account that x_i is a random variable with probability density $\varphi(x_i)$, the marginal density of y_i is

$$L(y_i,\underline{a}) = \int_{-\infty}^{\infty} L(y_i,\underline{a}|x_i)\, \varphi(x_i)\, dx_i .$$

We put $\varphi(x_i)$ from eq. /I.2.7/ and develop $f(x_i,\underline{a})$ in a power series around $x_i=x_{io}$, then we get after carrying out the integration that

$$L(y_i,\underline{a}) = \frac{1}{\sigma_i\sqrt{2\pi}} \exp\{-\frac{[y_i-f(x_{io},\underline{a})]^2}{2\sigma_i^2}\} \qquad /I.2.8a/$$

where

$$\sigma_i^2 = \sigma_{y_i}^2 + \sigma_{x_i}^2 \left[\frac{\partial f(x_{io},\underline{a})}{\partial x_i}\right]^2 . \qquad /I.2.8b/$$

We obtained that the modified distribution of y_i is also Gaussian but with an increased standard deviation: σ_{y_i} is replaced by σ_i given by eq. /I.2.8b/.

Let us now turn to the second case. Since vector $\underline{x}$ is random, the likelihood function defined in eq. /I.2.1/ has to be completed by the probability density of $\underline{x}$ i.e.

$$L(\underline{x},\underline{y},\underline{a}) = \frac{1}{(2\pi)^n \prod_{i=1}^{n} \sigma_{y_i}\sigma_{x_i}} \exp\{-\frac{1}{2}\sum_{i=1}^{n}\frac{[y_i-f(x_{io},\underline{a})]^2}{\sigma_{y_i}^2} - \frac{1}{2}\sum_{i=1}^{n}\frac{(x_i-x_{io})^2}{\sigma_{x_i}^2}\} .$$

According to the maximum likelihood principle, we have to search the maximum of logL as a function of $\underline{a}$ and $\underline{x}_o$. Differentiating logL with respect to a_k and x_{io} leads to the set of equations

$$\frac{\partial \log L}{\partial a_k} = \sum_{i=1}^{n} \frac{y_i-f(x_{io},\underline{a})}{\sigma_{y_i}^2} \frac{\partial f(x_{io},\underline{a})}{\partial a_k} = 0, \qquad /I.2.9a/$$

$$k = 1,2,\ldots,m$$

$$\frac{\partial \log L}{\partial x_{io}} = \frac{y_i-f(x_{io},\underline{a})}{\sigma_{y_i}^2} \frac{\partial f(x_{io},\underline{a})}{\partial x_{io}} + \frac{x_i-x_{io}}{\sigma_{x_i}^2} = 0. \qquad /I.2.9b/$$

$$i = 1,2,\ldots,n.$$

We develop $f(x_{io},\underline{a})$ in a power series around $x_{io} = x_i$:

$$f(x_{io},\underline{a}) = f(x_i,\underline{a}) - (x_i-x_{io})\frac{\partial f(x_i,\underline{a})}{\partial x_i}$$

which leads to

$$y_i - f(x_{io},\underline{a}) = y_i - f(x_i,\underline{a}) + (x_i-x_{io})\frac{\partial f(x_i,\underline{a})}{\partial x_i} . \qquad /I.2.10/$$

In eqs. /I.2.9/, we may substitute for derivatives $\frac{\partial f(x_{io},\underline{a})}{\partial a_k}$ and $\partial f(x_{io},\underline{a})/\partial x_i$ their values at x_i because this results in an error proportional to higher powers of (x_i-x_{io}) which were already neglected in eq.

/I.2.10/.In this way, our last formulae yield the following estimate for x_{io} from eq. /I.2.9b/:

$$x_i - \tilde{x}_{io} = - \frac{[y_i - f(x_i, \underline{a})] \frac{\partial f(x_i, \underline{a})}{\partial x_i}}{\left[\frac{\partial f(x_i, \underline{a})}{\partial x_i}\right]^2 + \frac{\sigma_{y_i}^2}{\sigma_{x_i}^2}} \quad . \qquad /I.2.11a/$$

In eq. /I.2.10/, this leads to

$$y_i - f(x_{io}, \underline{a}) = [y_i - f(x_i, \underline{a})] \frac{\sigma_{y_i}^2}{\sigma_{y_i}^2 + \sigma_{x_i}^2 \left[\frac{\partial f(x_i, \underline{a})}{\partial x_i}\right]^2} \quad .$$

If this expression is put in eq. /I.2.9a/, we obtain the final equations which contain only parameters a_k as unknowns:

$$\sum_{i=1}^{n} \frac{y_i - f(x_i, \underline{a})}{\sigma_i^2} \frac{\partial f(x_i, \underline{a})}{\partial a_k} = 0 \qquad /I.2.11b/$$

$$k = 1, 2, \ldots, m$$

where σ_i^2 is given by

$$\sigma_i^2 = \sigma_{y_i}^2 + \sigma_{x_i}^2 \left[\frac{\partial f(x_i, \underline{a})}{\partial x_i}\right]^2 \quad .$$

Eq. /I.2.11b/ is formally identical with eq. /I.2.5/ if weights w_i are derived from this σ_i^2 instead of $\sigma_{y_i}^2$.

Comparing our last expression for σ_i^2 with eq. /I.2.8b/, we see that the two cases considered here are really equivalent from the formal point of view. The only difference is that function $f(x_i, \underline{a})$ and its derivatives are calculated for x_{io} in the first case while for x_i in the second one. This is very convenient because these are just the values which are known in both cases.

As a conclusion, we state that x_i may be considered as a constant if its variance is incorporated in the weights according to eq. /I.2.8b/. When x_i is not a single variable, then it can be shown that each of its components contributes to σ_i^2 like $\sigma_{x_i}^2$ in eq. /I.2.8b/. We shall see examples of this in section V.1.

I.2.3 Poissonian distribution

Frequently, y_i is measured by a scaler so that its distribution is Poissonian. The corresponding likelihood function is given by eq. /I.1.5/. For not too small values of y_i /not less than about 100/, it is well approximated by a Gaussian distribution whose average and variance are both $f(x_i,\underline{a})$. In practical applications, it is quite general therefore to use the least squares method defined by eq. /I.2.4/ with a weighting

$$w_i = \frac{1}{y_i} \; . \qquad /I.2.12/$$

We ask how this approach is related to the maximum likelihood method. Putting $L(x_i,y_i,\underline{a})$ from eq. /I.1.5/ in eq. /I.1.4/, the likelihood equation /I.1.8/ reads as

$$\frac{\partial \log L(x,y,\underline{a})}{\partial a_k} = \sum_{i=1}^{n} \frac{y_i - f(x_i,\underline{a})}{f(x_i,\underline{a})} \frac{\partial f(x_i,\underline{a})}{\partial a_k} = 0. \qquad /I.2.13/$$

$$k = 1,2,\ldots,m$$

Comparison with eq. /I.2.5/ shows that this last equation corresponds to a weighting

$$w_i = \frac{1}{f(x_i,\underline{a})} \qquad /I.2.14/$$

but otherwise is formally identical with the equations of the least squares method. As the fitting assures that $y_i \approx f(x_i,\underline{a})$, the weighting defined by eq. /I.2.12/ is blameless if y_i is not small. It may be added that the solution of the set of equations /I.2.13/ does not strictly minimize the sum of squares in eq. /I.2.4/ if w_i is chosen according to eq. /I.2.14/.

It is advisable to put such a weighting option in a least squares fitting program. It is clear that this has more principal than practical significance since counts are almost always of the order of some thousands. In case of low counts, however, this is the only acceptable weighting. Let us suppose for example that function $f(x_i,\underline{a})$ is a decaying exponential plus a background, i.e.

$$f(x_i,\underline{a}) = a_1 e^{-a_2 x_i} + a_3$$

and the measurement is such that the y_i for large x_i are paractically constant. Mainly these last points will determine the background parameter a_3. It will be practically their average:

$$\tilde{a}_3 = \frac{\sum_i w_i y_i}{\sum_i w_i}$$

where the sum is extended for subscripts i for which $a_1 e^{-a_2 x_i} << a_3$. If w_i is chosen according to eq. /I.2.12/,

$$\tilde{a}_3 = \frac{n'}{\sum_i 1/y_i} \approx \frac{1}{\langle 1/y_i \rangle}$$

where n' is the number of y_i values considered here. For a Poissonian y_i with a_3 as mean, it may simply be shown that

$$\tilde{a}_3 \approx a_3 - 1 + \mathcal{O}(\frac{1}{a_3}) .$$

This means that a weighting according to eq. /I.2.12/ leads to a serious bias when a_3 is small. For example, this is 10 % when $a_3 = 10$. This difficulty is overcome by using weights according to eq. /I.2.14/.

I.2.4 Dead time correction in the maximum likelihood method

The finite time resolution of scalers leads to the so called dead time losses. The dead time correction may be very complicated in practical cases, expecially in case of time analyzers leading to rather frightening likelihood functions. A detailed analysis of time resolution problems is given e.g. in ref. [4]. Only the simplest and most frequent case will be studied here: the y_i are measured by a scaler which is insensitive to pulses during a time τ after the registration of a pulse. If the counting interval is T, usually, the correction factors

$$\nu_i = \frac{T}{T - y_i \tau} \qquad /I.2.15/$$

are applied to the registered counts y_i. It will be studied here how this approach fits in with the maximum likelihood method.

If the pulse rate is λ, the probability of counting k pulses in a time interval T is derived in ref. [1] as

$$P_k(\tau,T) \approx e^{-\lambda(T-k\tau)} \frac{[\lambda(T-k\tau)]^k}{k!} . \qquad /I.2.16/$$

/This approximation is valid if $\tau << T$./ Up to now, $f(x_i,\underline{a})$ was understood as the expectation of the total count so that, in our case,

$$\lambda = \frac{f(x_i,\underline{a})}{T} .$$

Therefore, $L(x_i,y_i,\underline{a})$ is now given by the formula

$$L(x_i,y_i,\underline{a}) = \exp\{-\frac{T-y_i\tau}{T} f(x_i,\underline{a})\} \frac{\left[\frac{T-y_i\tau}{T} f(x_i,\underline{a})\right]^{y_i}}{y_i!} . \qquad /I.2.17/$$

Inserting this in the maximum likelihood equation /I.1.8/, we get

$$\frac{\partial \log L(\underline{x},\underline{y},\underline{a})}{\partial a_k} = \sum_{i=1}^{n} \frac{\nu_i y_i - f(x_i,\underline{a})}{\nu_i f(x_i,\underline{a})} \frac{\partial f(x_i,\underline{a})}{\partial a_k} = 0. \qquad /I.2.18a/$$

$$k = 1,2,\ldots,m$$

We have found that the dead time correction factor ν_i is simply applied to y_i as it is usually done. But the question of the weighting needs some further study. We shall see that, if we carry out the dead time correction "by hand", give the resulting $\nu_i y_i$ values in input and consider them to be Poissonian, we make a slight error: the highest counts get higher weights than they ought to. Here, as everywhere else in the following, we rewrite eq. /I.2.18a/ in order to leave y_i alone and associate the correction with $f(x_i,\underline{a})$:

$$\sum_{i=1}^{n} \frac{y_i - f(x_i,\underline{a})/\nu_i}{f(x_i,\underline{a})/\nu_i} \frac{\partial f(x_i,\underline{a})/\nu_i}{\partial a_k} = 0. \qquad /I.2.18b/$$

$$k = 1,2,\ldots,m$$

In order to understand this weighting, let us calculate the expectation and variance of y_i. It is shown in Appendix 12* that for $\tau \ll T$

$$\langle y_i \rangle = \frac{f(x_i,\underline{a})}{1 + \frac{f(x_i,\underline{a})\tau}{T}} \approx \frac{f(x_i,\underline{a})}{\nu_i} \qquad /I.2.19/$$

and

$$\langle (\Delta y_i)^2 \rangle = \frac{f(x_i,\underline{a})}{\left[1+f(x_i,a)\frac{\tau}{T}\right]^3} \approx \frac{f(x_i,\underline{a})}{\nu_i^3} \approx \frac{y_i}{\nu_i^2}. \qquad /I.2.20/$$

It follows from these equations that the maximum likelihood method requires a weighting $1/y_i$ /the dead time correction is important only in case of high counts so that $y_i \approx \langle y_i \rangle$/. y_i is not, however, the variance of y_i but ν_i^2 times as large. Consequently, the correct weighting is not by reciprocal of the variance in this case.

When the variance of x_i is also taken into account, we have the following set of equations:

$$\sum_{i=1}^{n} \frac{y_i - f(x_i,\underline{a})/\nu_i}{y_i + \nu_i^2 \sigma_{x_i}^2 \left[\frac{1}{\nu_i} \frac{\partial f(x_i,\underline{a})}{\partial x_i}\right]^2} \frac{1}{\nu_i} \frac{\partial f(x_i,\underline{a})}{\partial a_k} = 0 \qquad /I.2.21/$$

$$k = 1,2,\ldots,m$$

*Formula /I.2.20/ was incorrectly given in the manuscript. It was Mr. Dupac /Prague University/ who gave to the author the correct expression on the basis of the renewal theory. The derivation of Appendix 12 is a direct calculation of the variance on the basis of ref. [1].

because the term containing $\sigma_{x_i}^2$ is added to the variance of y_i.

Up to now, we kept to the strict application of the maximum likelihood method. This led to a weighting which is not the reciprocal of the variance. The difference is factor ν_i^2 which, generally, does not exceed 1.10 to 1.15. If we neglect this, we use maximum 10 to 15 percent too high weights to some points. This is not at all terrible. The fact, however, that the denominator in eq. /I.2.21/ is not the variance of y_i would lead to difficulties in the study of the statistical properties of the solutions of the least squares equations. Therefore, we slightly deviate from eq. /I.2.21/ and will use the weighting

$$\frac{1}{w_i} = \frac{y_i}{\nu_i^2} + \sigma_{x_i}^2 \left[\frac{1}{\nu_i} \frac{\partial f(x_i,\underline{a})}{\partial x_i}\right]^2 \qquad /I.2.22a/$$

and the equation

$$G_k(\underline{a}) = \sum_{i=1}^{n} w_i \left[y_i - \frac{f(x_i,\underline{a})}{\nu_i}\right] \frac{1}{\nu_i} \frac{\partial f(x_i,\underline{a})}{\partial a_k} = 0. \qquad /I.2.22b/$$

$$k = 1,2,\ldots,m$$

The sum of squares is defined as

$$Q(\underline{a}) = \sum_{i=1}^{n} w_i \left[y_i - \frac{f(x_i,\underline{a})}{\nu_i}\right]^2 \qquad /I.2.22c/$$

which is analogous to eq. /I.2.4/.

I.3 Solution of the least squares equations

Set of equations /I.2.6/ may be solved by iteration. How this is done, it is outlined here only for the sake of completeness. We shall study only convergence problems in some detail. For simplicity, we consider the eventual dead time correction factors incorporated in $f(x_i,\underline{a})$.

Assume that ℓ iteration steps have already been accomplished resulting in $\underline{a}_\ell$. The next iterate $\underline{a}_{\ell+1}$ is determined in the following way. Developed $\underline{G}(\tilde{\underline{a}})$ in Taylor series around $\underline{a}_\ell$:

$$0 = \underline{G}(\tilde{\underline{a}}) = \underline{G}(\underline{a}_\ell) + \underline{\underline{D}}(\underline{a}_\ell)(\tilde{\underline{a}}-\underline{a}_\ell)+\ldots \qquad /I.3.1/$$

where the symmetric matrix $\underline{\underline{D}}$ is formed from the components

$$D_{kk'}(\underline{a}_\ell) = \frac{\partial G_k(\underline{a}_\ell)}{\partial a_{k'}} = -\frac{1}{2} \frac{\partial^2 Q(\underline{a}_\ell)}{\partial a_k \partial a_{k'}} . \qquad /I.3.2/$$

Solving eq. /I.3.1/ for $\tilde{\underline{a}}$ one gets $\underline{a}_{\ell+1}$ as

$$\underline{a}_{\ell+1} = \underline{a}_{\ell} - \underline{\underline{D}}^{-1}(\underline{a}_{\ell})\underline{G}(\underline{a}_{\ell}). \qquad /I.3.3a/$$

This iteration is terminated when $\underline{a}_{\ell}$ and $\underline{a}_{\ell+1}$ are sufficiently close to each other.

Eq. /I.2.6/ is usually transcendental and not easy to survey. It happens frequently, especially, when the number of the iterated parameters is more than 2, that the iteration diverges or converges to values which are trivially nonsense. For example, let us consider the function

$$f(x,\underline{a}) = a_1 \cos\left[a_2(x-a_3)\right].$$

When the initial guess $\underline{a}_o$ of the iteration is given in an unfortunate way, it happens sometimes that the iteration converges to the following "solution":

$$\begin{aligned} a_3 &= \text{anything}, \\ a_2 &= 0, \\ a_1 &= \bar{y} = \sum_{i=1}^{n} w_i y_i \Big/ \sum_{i=1}^{n} w_i \quad . \end{aligned}$$

This is quite nonsense from the physical point of view but not at all so from the mathematical point of view. The fact is that this a_1 is the correct solution of the following least squares problem:

$$Q(a_1) = \sum_{i=1}^{n} w_i (y_i - a_1)^2 = \text{minimum}.$$

On the plane $a_2 = 0$ of the paramter space, this apparent solution represents a real minimum of $Q(\underline{a})$. Of course, the physically meaningful solution leads to a much smaller minimum of Q than this. The point is only that the iteration does not find it.

Many procedures are known which aim at improving the original Newton iteration defined by eqs. /I.3.2/ and /I.3.3a/. We do not intend to study all of them but describe only that one which proved to work in a very stable way. Let us rewrite the iteration formula /I.3.3a/ as

$$\underline{a}_{\ell+1} = \underline{a}_{\ell} + \underline{\underline{M}}^{-1}(\underline{a}_{\ell})\underline{G}(\underline{a}_{\ell}) \qquad /I.3.3b/$$

where $\underline{\underline{M}}$ is an m by m symmetric matrix which will be specified later. Developing $Q(\underline{a}_{\ell+1})$ in a Taylor-series around $\underline{a}_{\ell}$, one can see how Q changes in an iteration step:

$$Q(\underline{a}_{\ell+1}) - Q(\underline{a}_\ell) = - 2\underline{G}^T(\underline{a}_\ell)(\underline{a}_{\ell+1}-\underline{a}_\ell) - (\underline{a}_{\ell+1}^T-\underline{a}_\ell^T)\,\underline{\underline{D}}(\underline{a}_\ell)(\underline{a}_{\ell+1}-\underline{a}_\ell)+\ldots$$

where eqs. /I.2.5/ and /I.3.2/ were used. Putting here $(\underline{a}_{\ell+1}-\underline{a}_\ell)$ from eq. /I.3.3b/, we get

$$Q(\underline{a}_{\ell+1}) - Q(\underline{a}_\ell) =$$

$$= -\underline{G}^T(\underline{a}_\ell)\underline{\underline{M}}^{-1}(\underline{a}_\ell)\underline{G}(\underline{a}_\ell) - \underline{G}^T(\underline{a}_\ell)\underline{\underline{M}}^{-1}(\underline{a}_\ell)\left[\underline{\underline{D}}(\underline{a}_\ell)+\underline{\underline{M}}(\underline{a}_\ell)\right]\underline{\underline{M}}^{-1}(\underline{a}_\ell)\underline{G}(\underline{a}_\ell)+\ldots \qquad /I.3.4/$$

If $\underline{\underline{M}}(\underline{a}_\ell)$ is chosen such that it is as close as possible to $-\underline{\underline{D}}(\underline{a}_\ell)$ and it is a positive definite matrix, then $Q(\underline{a}_{\ell+1})$ will be less than $Q(\underline{a}_\ell)$, consequently the iteration will proceed towards the minimum of $Q(\underline{a})$. Of course, when $\underline{a}_\ell$ is so far from the minimum that the higher order terms may not be neglected in eq. /I.3.4/, even this trick does not garantee that $Q(\underline{a}_{\ell+1})<Q(\underline{a}_\ell)$. When the iteration matrix is $-\underline{\underline{D}}$ /as in eq. /I.3.3a//, then eq. /I.3.4/ reads as

$$Q(\underline{a}_{\ell+1}) - Q(\underline{a}_\ell) = \underline{G}^T(\underline{a}_\ell)\underline{\underline{D}}^{-1}(\underline{a}_\ell)\underline{G}(\underline{a}_\ell) + \ldots$$

Matrix $\underline{\underline{D}}(\underline{a}_\ell)$ is negativ definite only near the minimum. That is why the Newton iteration is unstable when the initial guess is relatively far from the solution. It is also true, however, that once near the minimum, $\underline{\underline{D}}(\underline{a}_\ell)$ is the best iteration matrix. Therefore, $\underline{\underline{M}}$ may not be very different from $-\underline{\underline{D}}$.

Let us calculate matrix elements $D_{kk'}$, explicitely:

$$D_{kk'}(\underline{a}_\ell) = -\sum_{i=1}^{n} w_i \frac{\partial f(x_i,\underline{a}_\ell)}{\partial a_k}\frac{\partial f(x_i,\underline{a}_\ell)}{\partial a_{k'}} + \sum_{i=1}^{n} w_i\left[y_i-f(x_i,\underline{a}_\ell)\right]\frac{\partial^2 f(x_i,\underline{a}_\ell)}{\partial a_k\,\partial a_{k'}}\,.$$

The first sum here is the element of a positive definite matrix /as it may be simply shown/, while the second sum vanishes on the average. Thus, the choice

$$M_{kk'}(\underline{a}_\ell) = \sum_{i=1}^{n} w_i \frac{\partial f(x_i,\underline{a}_\ell)}{\partial a_k}\frac{\partial f(x_i,\underline{a}_\ell)}{\partial a_{k'}} \qquad /I.3.5/$$

$$k,k' = 1,2,\ldots,m$$

meets what was required from it earlier.

Practice has shown that this matrix assures convergence for a vast variety of initial guesses. Apart from this, the computation of $\underline{\underline{M}}$ is approximately m^2 times as fast as that of $\underline{\underline{D}}$.

CHAPTER II.

STATISTICAL PROPERTIES OF THE ESTIMATES

In the previous chapter, the question of calculating estimate vector $\underline{\tilde{a}}$ was treated. This and the following sections will be devoted to the analysis of its statistical properties. Our derivations mainly follow the lines of ref. [2].

As it was stated in section II.1, $\underline{\tilde{a}}$ may be assumed as a Gaussian random variable. Consequently, its behaviour is fully characterized by its average and its covariance matrix.

II.1 Covariance matrix

It will be expedient to introduce some notations. Derivatives $\frac{\partial f(x_i,\underline{a})}{\partial a_k}$ will be considered as the elements of matrix $\underline{\underline{F}}$:

$$F_{ik} = \frac{\partial f(x_i,\underline{a})}{\partial a_k} \quad . \qquad /II.1.1/$$

$$i = 1,2,\ldots,n$$
$$k = 1,2,\ldots,m$$

From weights w_i, we form the diagonal matrix $\underline{\underline{W}}$:

$$W_{ii} = w_i . \qquad /II.1.2/$$

According to eqs. /I.2.2/ and /I.2.3/, the covariance matrix of measurement vector $\underline{y}$ may be written as

$$<\Delta y \Delta y^T> = \sigma^2 \underline{\underline{W}}^{-1} \quad . \qquad /II.1.3/$$

In these notations, matrix $\underline{\underline{M}}$ defined by eq. /I.3.5/ is expressed in the form

$$\underline{\underline{M}} = \underline{\underline{F}}^T \underline{\underline{W}} \underline{\underline{F}} \quad . \qquad /II.1.4/$$

The expectation of y_i will be denoted by

$$\langle y_i \rangle = \eta_i . \qquad /II.1.5/$$

In the basic equation /I.2.6/, only one argument was explicitly indicated in $\underline{G}$ while, in reality, there is another one, namely $\underline{y}$. Therefore, eq. /I.2.6/ is rewritten as

$$\underline{G}(\underline{y},\underline{\tilde{a}}) = 0 \qquad /II.1.6/$$

which emphasizes the dependence of $\underline{\tilde{a}}$ on $\underline{y}$.

In section I.1, we assumed that there is no systematic error in the measurement, so that $\underline{\eta}$ and the true parameter vector $\underline{a}$ satisfy this equation, i.e.

$$\underline{G}(\underline{\eta},\underline{a}) = 0.$$

Setting

$$\Delta y_i = y_i - \eta_i \qquad /II.1.7a/$$

and

$$\Delta a_k = \tilde{a}_k - a_k , \qquad /II.1.7b/$$

develop $\underline{G}(\underline{y},\underline{\tilde{a}})$ in a power series around $(\underline{\eta},\underline{a})$:

$$0 = \sum_{i=1}^{n} \frac{\partial G_k(\underline{\eta},\underline{a})}{\partial y_i} \Delta y_i + \sum_{k'=1}^{m} \frac{\partial G_k(\underline{\eta},\underline{a})}{\partial a_{k'}} \Delta a_{k'} +$$

$$+ \frac{1}{2} \sum_{k'=1}^{m} \sum_{k''=1}^{m} \frac{\partial^2 G_k(\underline{\eta},a)}{\partial a_{k'}\, \partial a_{k''}} \Delta a_{k'} \Delta a_{k''} + \ldots \qquad /II.1.8/$$

Using eq. /I.2.5/, it may be seen that

$$\frac{\partial G_k(\underline{\eta},\underline{a})}{\partial y_i} = w_i F_{ik} = \{\underline{\underline{F}}^T \underline{\underline{W}}\}_{ki} \qquad /II.1.9/$$

and

$$\frac{\partial G_k(\underline{\eta},\underline{a})}{\partial a_{k'}} = - \{M\}_{kk'} . \qquad /II.1.10/$$

The double derivatives of G_k are considered as the elements of matrix $-\underline{\underline{H}}_k$:

$$\frac{\partial^2 G_k(\underline{\eta},\underline{a})}{\partial a_{k'}\, \partial a_{k''}} = - \{\underline{\underline{H}}_k\}_{k'\,k''} \qquad /II.1.11/$$

It was neglected here that the weights may depend on y_i and $\underline{a}$. This dependence, however, leads to higher order corrections which may surely be neglected. The third sum in eq. /II.1.8/ is significant only when $f(x_i,\underline{a})$ is highly nonlinear in $\underline{a}$. If it is neglected, eq. /II.1.8/ may be put in vector form:

$$\underline{\underline{F}}^T \underline{\underline{W}} \Delta\underline{y} - \underline{\underline{M}} \Delta\underline{a} = 0$$

or

$$\Delta\underline{a} = \underline{\underline{M}}^{-1} \underline{\underline{F}}^T \underline{\underline{W}} \Delta\underline{y}. \qquad /II.1.12/$$

Taking the average of both sides, $\langle\Delta\underline{a}\rangle=0$ results i.e. estimate vector $\tilde{\underline{a}}$ is unbiased when $f(x_i,\underline{a})$ is linear in $\underline{a}$. In case of a nonlinear function $f(x_i,\underline{a})$, however, the neglected second order term of eq. /II.1.8/ may lead to a bias. This will be studied in the next section. For the purpose of calculating the covariance matrix of $\tilde{\underline{a}}$, eq. /II.1.12/ is sufficient.

The covariance matrix is by definition

$$\underline{\underline{B}} = \langle\Delta\underline{a}\ \Delta\underline{a}^T\rangle$$

which may be easily calculated by using eq. /II.1.12/. The result is

$$\underline{\underline{B}} = \sigma^2\underline{\underline{M}}^{-1}. \qquad /II.1.13/$$

This is a well known formula. Some fitting programs use matrix $-\underline{\underline{D}}$ /see eq. /I.3.2// instead of $\underline{\underline{M}}$. The diagonal elements of $\underline{\underline{B}}$ give the variances of parameter estimates $\tilde{a}_k$.

Eq. /II.1.13/ is only a first order approximation of $\underline{\underline{B}}$ for several reasons. First, it was obtained by neglecting the second order term in eq. /II.1.8/. This results in an error of the order of σ^4 as it will be shown in the next section. Second, the dependence of the weights on y_i and $\underline{a}$ results in also an error of order σ^4. Finally, $\underline{\underline{M}}$ ought to be calculated for $\underline{a}$ but we can calculate it only for $\tilde{\underline{a}}$. This also leads to an error of the same order.

At first sight, it may be unusual that we declare terms proportional to σ^4 small with respect to terms proportional to σ^2 without proving that σ^2 is small. The fact is that σ^2 is really a measure of the accuracy of the given measurement. If the weights are normalized in some way /e.g. $\sum_{i=1}^{n} w_i = 1$ is set/, the accurate measurements are characterized by a small σ^2, inaccurate measurements by a large one. In this sense, this "series expansion" is not convergent only for very inaccurate measurements.

II.2 Average

It was seen in the previous section that $\tilde{\underline{a}}$ is an unbiased estimate if the second order term in eq. /II.1.8/ may be neglected. We study now the consequences of the appearence of this term. Let $\underline{h}$ be a vector with components

$$h_k = \Delta\underline{a}^T \underline{\underline{H}}_k \Delta\underline{a} \ . \qquad /II.2.1/$$

We have now instead of eq. /II.1.12/ that

$$\Delta\underline{a} = \underline{\underline{M}}^{-1}(\underline{\underline{F}}^T \underline{\underline{W}} \Delta\underline{y} - \tfrac{1}{2}\underline{h}). \qquad /II.2.2/$$

Taking the expectation of both sides, we get:

$$\delta\underline{a} = \langle\Delta\underline{a}\rangle = -\tfrac{1}{2}\underline{\underline{M}}^{-1} \langle\underline{h}\rangle \qquad /II.2.3/$$

where $\delta\underline{a}$ is the bias of estimate $\tilde{\underline{a}}$. This relation is an equation for $\delta\underline{a}$ because $\langle\underline{h}\rangle$ depends on $\delta\underline{a}$. From eq. /II.2.1/, it may be easily obtained that

$$\langle h_k \rangle = \delta\underline{a}^T \underline{\underline{H}}_k \delta\underline{a} + \sigma^2 \sum_{k'=1}^{m} \{\underline{\underline{M}}^{-1} \underline{\underline{H}}_k\}_{k'k'} \ .$$

When this is put in eq. /II.2.3/, we get the following set of equations:

$$\{\underline{\underline{M}}\delta\underline{a}\}_k = -\tfrac{1}{2}\delta\underline{a}^T \underline{\underline{H}}_k \delta\underline{a} - \frac{\sigma^2}{2} \sum_{k'=1}^{m} \{\underline{\underline{M}}^{-1} \underline{\underline{H}}_k\}_{k'k'} \ . \qquad /II.2.4/$$

$$k = 1,2,\ldots,m$$

Thus we have got a set of quadratic equations for components δa_k which may be solved by iteration or otherwise. It is not worthwhile, however, to solve it exactly. The fact is that it is valid to an order of σ^2, therefore, it is sufficient to find the leading term of its solution. Hence the first term on the right hand side may be neglected because it is of order σ^4. This simplified equation may be written as follows. Let g_k be

$$g_k = \sum_{k'=1}^{m} \{\underline{\underline{M}}^{-1} \underline{\underline{H}}_k\}_{k'k'} \qquad /II.2.5/$$

and form vector $\underline{g}$ from these components. Then we have from eq. /II.2.4/

$$\delta\underline{a} = -\frac{\sigma^2}{2} \underline{\underline{M}}^{-1}\underline{g}. \qquad /II.2.6/$$

This is also a first order expression. It is remarkable that the bias is proportional to σ^2 while the standard deviations of the parameters are proportional to σ as eq. /II.1.13/ shows. Therefore, the bias may be

expected to be small in normal cases. There may be, however, cases in which this bias plays an important role. In any case, we do not lose anything by correcting for it. The corrected estimate

$$\underline{a}^* = \tilde{\underline{a}} - \delta\underline{a} \qquad /II.2.7/$$

is unbiased to the order of σ^4:

$$<\underline{a}^*> = \underline{a} + \mathcal{O}(\sigma^4).$$

It is important to remark that the calculation of the bias, especially the calculation of matrices $\underline{\underline{H}}_k$ is rather time consuming. The necessary computing time is roughly proportional to m^3. As a rule, this calculation requires as much time as the iteration.

We have left to study how the appearence of the bias influences formula /II.1.13/ derived for the covariance matrix. The true covariance matrix would be

$$\underline{\underline{B}}^* = <(\tilde{\underline{a}}-<\tilde{\underline{a}}>)(\tilde{\underline{a}}^T-<\tilde{\underline{a}}^T>)> = <(\Delta\underline{a}-\delta\underline{a})(\Delta\underline{a}^T-\delta\underline{a}^T)> =$$

$$= <\Delta\underline{a}\Delta\underline{a}^T> - \delta\underline{a}\delta\underline{a}^T = \underline{\underline{B}} - \delta\underline{a}\delta\underline{a}^T. \qquad /II.2.8/$$

Thus, the difference in $\underline{\underline{B}}$ is $\delta\underline{a}\delta\underline{a}^T$ which is of the order of σ^4 as anticipated in the previous section. Other terms of this order have already been neglected. Therefore, it is proper to do the same now.

The role of the bias is illustrated by numerical examples. Table II.1 shows the results of the fitting for cases 1 to 3 /see Appendix 10/.

Table II.1

case	$\tilde{a}_1 \pm \Delta\tilde{a}_1$ (δa_1)	$(\tilde{a}_2 \pm\Delta\tilde{a}_2)\cdot 10^2 (\delta a_2 \cdot 10^2)$	$\tilde{a}_3 \pm \Delta\tilde{a}_3 \pm (\delta\tilde{a}_3)$
1	9980.95 ± 17.27(-0.37)	2.023 ± 0.018($6\cdot 10^{-4}$)	30.48 ± 0.39(0.017)
2	994.04 ± 6.16(-0.51)	2.024 ± 0.065($8\cdot 10^{-3}$)	30.34 ± 1.42(0.22)
3	106.17 ± 3.92(-2.17)	1.683 ± 0.216(0.090)	16.12 ± 8.49(4.81)

Here, case 1 represents a typically accurate measurement. The bias is at least by an order of magnitude less than the statistical error of parameter estimates. For the most important parameter i.e. for a_2 /the axial buckling/, it is about 3 % of $\Delta\tilde{a}_2$. Practice has shown that most real measurements show a similar behaviour of the bias, consequently, it may generally be neglected.

The best policy which can be recommended is that, for each type of measurement, at least one typical case has to be studied from the point of view of the bias. If it behaves as in case 1, neglect it for all similar measurements, if as in case 2, correct for it according to eq. /II.2.7/, and if as in case 3, try to repeat the measurement with a significantly better accuracy.

In chapter IV, the point drop technique of evaluation will be treated in which the set of values y_i is reduced step by step. From step to step, the statistical errors of the parameter estimates increase but so do the biases. Table II.2 shows this for case 1. It may be concluded that the bias increases somewhat faster than the error so that it may become important in later steps. As it will be shown in chapter IV, the ratios

$$\delta t_\ell = \frac{\delta a_k^{\ell+1} - \delta a_k^{\ell}}{\sqrt{(\Delta\tilde{a}_k^{\ell+1})^2 - (\Delta\tilde{a}_k^{\ell})^2}}$$

are of interest where superscript ℓ refers to quantities obtained in step ℓ. These ratios are also given in Table II.2.

Table II.2

ℓ	(x_{first}, x_{last})	$(\tilde{a}_2 \pm \Delta\tilde{a}_2)\cdot 10^2$	$\delta a_2 \cdot 10^2$	δt_ℓ
1	19,82	2.0233 ± 0.0184	$5.82\cdot 10^{-4}$	0.0221
2	21,80	2.0105 ± 0.0223	$8.60\cdot 10^{-4}$	0.0273
3	23,78	2.0156 ± 0.0273	$1.29\cdot 10^{-3}$	0.0363
4	25,76	1.9931 ± 0.0339	$2.02\cdot 10^{-3}$	0.0491
5	27,74	1.9860 ± 0.0429	$3.31\cdot 10^{-3}$	0.0696
6	29,72	1.9607 ± 0.0545	$5.65\cdot 10^{-3}$	0.0997
7	31,70	1.9879 ± 0.0695	$9.95\cdot 10^{-3}$	0.2220
8	33,68	2.0167 ± 0.0934	$2.38\cdot 10^{-2}$	0.554
9	35,66	2.1829 ± 0.1110	$5.70\cdot 10^{-2}$	

As it will be shown in chapter IV, the bias is negligible if $\delta t_\ell << 1$. This is by far not true for the last steps in this concrete example. A general recipe can hardly be given as to when the bias is really negligible. Therefore, it is recommended to prepare such a table for a typical measurement and to decide on its basis whether to take it into account or to neglect it or whether the measurements at hand are too inaccurate and ought to be repeated.

II.3 Estimation of σ^2

In our previous formulae, parameter σ^2 occured frequently. According to eq. /I.2.3/, it characterizes the accuracy of the measurements. It is not surprising therefore that the accuracies of the parameter estimates also depend on it. Formulae like /II.1.13/ or /II.2.6/ are useless unless we are able to give an estimate for σ^2. This is generally based on the following theorem. The minimum value Q_{min} of the sum of squares $Q(\underline{a})$ has the property that

$$Q_{min} = \sigma^2 \chi^2_{n-m} \ . \qquad /II.3.1/$$

A proof of this basic theorem is not given here, it may be found e.g. in ref [2].

As the expectation of χ^2_{n-m} is /n-m/, therefore the expression

$$\tilde{\sigma}^2 = \frac{Q_{min}}{n-m} \qquad /II.3.2/$$

may be used as an unbiased estimate of σ^2. Putting this in eq. /II.1.13/, the final formula for the standard deviations $\Delta\tilde{a}_k$ is obtained:

$$\Delta\tilde{a}_k = \sqrt{\{\underline{\underline{B}}\}_{kk}} = \frac{Q_{min}}{n-m} \{\underline{\underline{M}}^{-1}\}_{kk} \ . \qquad /II.3.3/$$

$$k = 1,2,\ldots,m$$

Eq. /II.3.2/ is a generally accepted formula. As usually happens, the applicability of even the most powerful theoretical results depends on a number of conditions. It is not without interest therefore to say a few words on the problems connected with the application of this formula.

The proof given by ref. [2] assumes that eq. /II.1.12/ is valid i.e. it considers $\tilde{\underline{a}}$ unbiased. It is clear from this that eq. /II.3.1/ is only a first order approximation, its error being of the order of σ^4. Such errors were already neglected in $\underline{\underline{B}}$ /cf. eq. /II.2.8// so that we have to tolerate it here, too.

The variance of χ^2_{n-m} is relatively large, namely 2(n-m). The relative error of $\tilde{\sigma}^2$ is therefore $\sqrt{2/(n-m)}$ which ranges from 10 to 50 percents in practical cases. When estimates $\tilde{a}_k$ are compared to calculations, the generally accepted Gaussian criteria /e.g. the "3σ" confidence interval/ are false. A Student test is to be preferred as described in chapter III.

Eq. /II.3.1/ is valid only under the assumption that function $f(x_i,\underline{a})$ fits well the whole range of points x_i. Even a small range of "bad" points leads to a serious overestimation of σ^2 when using eq. /II.3.2/. It will be the subject of chapters III. and IV. how such a kind of discrepancy can be detected.

Sometimes, eq. /II.3.1/ is used not to estimate σ^2 but to check the goodness of fit. The phylosophy is that the weighting factors w_i are carefully chosen to be $1/\sigma_i^2$ /cf. ew. /I.2.3//, consequently, $\sigma^2 = 1$ may be assumed. Under this assumption, eq. /II.3.1/ may really be the basis of a χ^2 test of the goodnes of fit. The present paper does not subscribe to this practice. The fact is that it is practically impossible to asses all possible sources of error and include them in σ_i^2 with such an assurance that eq. /II.3.1/ might be the basis of a test of goodness of fit. The main point of estimating σ^2 by eq. /II.3.2/ is juste that we account by it for some hidden sources of error.

The question may now be raised: why did we suppose in eq. /I.2.3/ that the hidden errors change σ_i^2 in a <u>proportional</u> way? Why did not we <u>add</u> something to it? One must acknowledge that the question is justified. We have seen in section I.2.2 that, for example, the error in x_i leads to an additive term /cf. eq. /I.2.11// which is by no means proportional to σ_y^2. The main reason of introducing improvements such as eq. /I.2.11/ was to keep eq. /I.2.3/ as valid as possible. Most of other sources of error which can not be taken into account by formulae like eq. /I.2.11/ may really be assumed to satisfy eq. /I.2.3/ i.e. the assumption of proportionality. For example, the uncertainty of positioning a foil on the tray under the scintillation counter may be assumed to result in a change of the count proportional to it. Nevertheless, eq. /I.2.3/ remains an approximation.

Finally, it may not be expected that crude errors of measurement /such as a mistaken record of a count, e.g. by a bad analyzer channel/ are corrected for by $\tilde{\sigma}^2$ as given by eq. /II.3.2/. Such an error leads to a serious bias in $\underline{\tilde{a}}$ and a strong overestimation of its standard deviation. It can be frequently heard to say that so broad a confidence interval may be obtained in this way that is surely contains the true parameter value $\underline{a}$. If one looks at it carefully, one sees that it is a strong violation of our basic assumptions. Thus the resulting "confidence interval" will be certainly an interval but without any confidence. Such bad points must be picked up by the evaluation procedure and then rejected. It will be treated in chapter III. how to achieve this.

II.4 Estimation of $\langle y_i \rangle$

After having obtained parameter estimate $\underline{\tilde{a}}$, one usually calculates the values of the fitted function $f(x_i, \underline{\tilde{a}})$. This "smooth" curve is then compared to the "fluctuating" curve which is drawn using the measured values y_i. The purpose of this is to check both the goodness of fit and the measured values point by point. In case of a good fit and a good measurement, the approximate equality

$$y_i \approx \tilde{y}_i = f(x_i, \underline{\tilde{a}}) \qquad /II.4.1/$$

may be expected to hold. How well it may be required to hold, this question may be answered only on the basis of the statistical properties of $\tilde{y}_i$. These latter are the subject of the present section while the problem of the equality $y_i \approx \tilde{y}_i$ will be studied in section III.2.

If $\langle\tilde{y}_i\rangle = \langle y_i\rangle = f(x_i, \underline{a})$ holds, $\tilde{y}_i$ is an unbiased estimate of $\langle y_i\rangle$. This can be true only for a function $f(x_i, \underline{a})$ linear in $\underline{a}$ if otherwise $\underline{\tilde{a}}$ is an unbiased estimate of $\underline{a}$. In section II.2, it was shown that this latter requirement is met only for a linear function. Therefore, $\tilde{y}_i$ is biased in the general case. Let us expand $f(x_i, \underline{\tilde{a}})$ in a power series around $\underline{a}$:

$$\tilde{y}_i = f(x_i, \underline{a}) + \sum_{k=1}^{m} \frac{\partial f(x_i, \underline{a})}{\partial a_k} \Delta a_k + \frac{1}{2} \sum_{k=1}^{m} \sum_{k'=1}^{m} \frac{\partial^2 f(x_i, \underline{a})}{\partial a_k \partial a_{k'}} \Delta a_k \Delta a_{k'} + \ldots \qquad /II.4.2/$$

where Δa_k was defined by eq. /II.1.7b/. Taking the expectation value of both sides of this equation, we get the bias δy_i:

$$\delta y_i = \langle\tilde{y}_i\rangle - f(x_i, \underline{a}) =$$

$$= \sum_{k=1}^{m} \frac{\partial f(x_i, \underline{a})}{\partial a_k} \delta a_k + \frac{1}{2} \sum_{k=1}^{m} \sum_{k'=1}^{m} \frac{\partial^2 f(x_i, \underline{a})}{\partial a_k \partial a_{k'}} \{\underline{\underline{B}}\}_{kk'} + \Theta(\sigma^4) \qquad /II.4.3/$$

where δa_k is the bias of the parameter estimate /see eq. /II.2.6// and $\underline{\underline{B}}$ is the covariance matrix given by eq. /II.1.13/. From the considerations of section II.2, it follows that the neglected higher order terms are of the order of at least the fourth power of σ. Consequently,

$$y_i^* = \tilde{y}_i - \delta y_i = f(x_i, \underline{\tilde{a}}) -$$

$$- \sum_{k=1}^{m} \frac{\partial f(x_i, \underline{\tilde{a}})}{\partial a_k} \delta a_k - \frac{1}{2} \sum_{k=1}^{m} \sum_{k'=1}^{m} \frac{\partial^2 f(x_i, \underline{\tilde{a}})}{\partial a_k \partial a_{k'}} \{\underline{\underline{B}}\}_{kk'} \qquad /II.4.4/$$

may be considered as an unbiased estimate of $\langle y_i\rangle$ because

$$\langle y_i^*\rangle = f(x_i, \underline{a}) + \Theta(\sigma^4). \qquad /II.4.5/$$

In practical cases, correction δy_i is small but it costs very little to take it into account. It is relatively large only for very inaccurate measurements i.e. when σ^2 is large.

We turn now to the calculation of the covariance matrix of y_i^*. This will be calculated only in first approximation i.e. we shall neglect the bias. The covariance matrices of y_i^*, and $\tilde{y}_i$ differ only to $\theta(\sigma^4)$. We may then write from eq. /II.4.2/ that

$$\Delta\tilde{y}_i = \tilde{y}_i - f(x_i,\underline{a}) = \{\underline{\underline{F}}\Delta\underline{a}\}_i \qquad /II.4.6/$$

where matrix $\underline{\underline{F}}$ has been defined by eq. /II.1.1/. Forming vector $\Delta\underline{\tilde{y}}$ from components $\Delta\tilde{y}_i$, the covariance matrix is given by

$$<\Delta\underline{\tilde{y}}\Delta\underline{\tilde{y}}^T> = \underline{\underline{F}}<\Delta\underline{a}\Delta\underline{a}^T>\underline{\underline{F}}^T = \underline{\underline{F}}\underline{\underline{B}}\underline{\underline{F}}^T = \sigma^2\underline{\underline{F}}\underline{\underline{M}}^{-1}\underline{\underline{F}}^T. \qquad /II.4.7/$$

Taking the diagonal elements of this matrix, we estimate the variance of $\tilde{y}_i$ or y_i^*:

$$\sigma_i^{*2} = \tilde{\sigma}^2\{FM^{-1}F^T\}_{ii} \qquad /II.4.8/$$

where $\tilde{\sigma}^2$ is the estimate of σ^2 as given by eq. /II.3.2/.

Finally, the variance of y_i can be estimated on the basis of eq. /I.2.3/:

$$\tilde{\sigma}_i^2 = \frac{\tilde{\sigma}^2}{w_i} . \qquad /II.4.9/$$

In this way, a succesful fitting gives an idea concerning the accuracy of our original measurements. This is, of course, a complicated quantity. It contains several components:

- component $\sigma_{y_i}^2$ which we could asses a priori /e.g. if y_i is Poissonian, $\sigma_{y_i}^2 \approx y_i$/,
- a component due to that x_i is random /cf. the term containing σ_x^2 in eq. /I.2.8b/.
- and finally, hidden error components which could not be assesed in either of these previous two ways; this is represented by $\tilde{\sigma}^2$.

When we compare our measured curve to some calculated curve, all these error components should be taken into account. In other words, the standard deviation given by eq. /II.4.9/ should be used.

II.5 Further statistical properties of the estimates

In the following sections, we shall need a further property of estimate $\tilde{\underline{a}}$: vector $(y-\tilde{y})$ is statistically independent of $\tilde{\underline{a}}$ /of course, neglecting terms of $\theta(\sigma^4)$.

The proof of this statement is rather simple. We have seen that

$\langle y_i \rangle = \langle \tilde{y}_i \rangle = f(x_i, \underline{a})$ when the bias is neglected. Therefore, in view of eqs. /II.4.6/ and /II.1.12/, we may write that

$$\underline{y} - \tilde{\underline{y}} = \Delta\underline{y} - \Delta\tilde{\underline{y}} = \Delta\underline{y} - \underline{\underline{F}}\Delta\underline{a} = \Delta\underline{y} - \underline{\underline{F}}\underline{\underline{M}}^{-1}\underline{\underline{F}}^{T}\underline{\underline{W}}\Delta\underline{y}. \qquad /II.5.1/$$

The covariance matrix of $(\underline{y}-\tilde{\underline{y}})$ and $\tilde{\underline{a}}$ is by definition

$$\langle(\underline{y}-\tilde{\underline{y}})\Delta\underline{a}^{T}\rangle = \langle(\Delta\underline{y}-\underline{\underline{F}}\underline{\underline{M}}^{-1}\underline{\underline{F}}^{T}\underline{\underline{W}}\Delta\underline{y})\ \Delta\underline{y}^{T}\underline{\underline{W}}\underline{\underline{F}}\underline{\underline{M}}^{-1}\rangle =$$

$$= \sigma^2\underline{\underline{F}}\underline{\underline{M}}^{-1} - \sigma^2\underline{\underline{F}}\underline{\underline{M}}^{-1}\underline{\underline{F}}^{T}\underline{\underline{W}}\underline{\underline{F}}\underline{\underline{M}}^{-1} = \sigma^2\underline{\underline{F}}\underline{\underline{M}}^{-1} - \sigma^2\underline{\underline{F}}\underline{\underline{M}}^{-1} = 0 \qquad /II.5.2/$$

where eqs. /II.1.3/ and /II.1.4/ were taken into account. /If we had not neglected the bias, we would have obtained $\Theta(\sigma^4)$ instead of zero for the covariance matrix./ Since all random variables here are considered to be Gaussian, vanishing of the convariances means statistical independence. This proves our statement.

This property has some interesting corollaries:

a/ Vector $(\underline{y}-\tilde{\underline{y}})$ is independent of $\tilde{\underline{y}}$, the latter being a function of $\tilde{\underline{a}}$ /see eq. /II.4.6//.

b/ Q_{min} is independent of both $\tilde{\underline{a}}$ and $\tilde{\underline{y}}$ because Q_{min} is the sum of terms $w_i(\tilde{y}_i-\tilde{y}_i)^2$ and each of them is independent of both $\tilde{\underline{a}}$ and $\tilde{\underline{y}}$.

A more detailed study of the statistical behaviour of the least square estimates may be found in ref. [2]. In this reference like the other ones known to the author, however, nothing is written about the biases $\delta\underline{a}$ and $\delta\underline{y}$. That is why this paper devoted so much place to the study of the problems connected with the bias.

CHAPTER III.

INTERVAL ESTIMATES

Measurements are carried out mainly in order to check the validity of some theoretical predictions. This can be done either on the level of the "measured curve" i.e. the graphic plot of the values y_i is compared to a theoretical curve or on the level of parameters a_k i.e. the parameter estimates are compared to the calculated values. In both cases, the problem may be formulated as follows: we test the hypothesis H_o that the calculated values agree with the expectations of the measured and/or estimated values. The alternative hypothesis H_1 against which the test is made is the disagreement.

In some cases, there is no calculated value and the purpose of the measurement and evaluation is the determination of some or all of parameters a_k. Even in this case, it is necessary to check the goodness of fit. In this chapter and in chapter IV, two procedures are suggested. The present one treats a pointwise test which aims at detecting crude experimental errors or some unexpected deviation of $\langle y_i \rangle$ from $f(x_i, \underline{a})$. Chapter IV suggests a global method which helps to find those regions of x_i in which $f(x_i, \underline{a}) = \langle y_i \rangle$ holds. This latter can be used, however, only when we have already some a priori idea concerning the studied discrepancies.

III.1 Parameter estimation using confidence intervals

Result $\tilde{\underline{a}}$ of the least squares fitting is a point estimate. When it is compared to calculated values, the question of agreement or disagreement can be decided only by taking the variance into account. The corresponding confidence interval is usually determined in the following way.

Parameter estimate $\tilde{a}_k$ has a standard deviation according to eq. /II.3.3/. This itself is an estimate while the true one is $\sigma\sqrt{\{M^{-1}\}_{kk}}$ /see eq. /II.1.13//. Thus, we know that

$$\xi = \frac{a_k^* - a_k}{\sigma\sqrt{\{\underline{\underline{M}}^{-1}\}_{kk}}} \qquad /III.1.1/$$

is N(0,1). Eq. /II.3.1/ tells us that Q_{min}/σ^2 is equal to χ^2_{n-m}. We proved in section II.5 that it is independent of $(a_k^*-a_k)$ and, consequently, of ξ too. This allows to combine $(a_k^*-a_k)$ and $\Delta\tilde{a}_k$ to a Student fraction

$$t = \frac{\xi}{\sqrt{\frac{\chi^2_{n-m}}{n-m}}} = \frac{a_k^* - a_k}{\sigma\sqrt{\{\underline{\underline{M}}^{-1}\}_{kk}}} \frac{1}{\sqrt{\frac{Q_{min}}{\sigma^2(n-m)}}} = \frac{a_k^* - a_k}{\Delta\tilde{a}_k} . \qquad /III.1.2/$$

/As a rule, number (n-m) of degrees of freedom is indicated at t as a subscript but we omitted it in order to avoid too complicated notations later./ Suppose that a confidence probability ε is chosen and determine quantile γ such that

$$P\{|t| < \gamma\} = 1 - \varepsilon. \qquad /III.1.3/$$

Putting in here expression /III.1.2/ for t, we may state that the true parameter value a_k satisfies the unequalities

$$a_k^* - \gamma\Delta\tilde{a}_k < a_k < a_k^* + \gamma\Delta\tilde{a}_k \qquad /III.1.4/$$

with probability $(1-\varepsilon)$. Tables giving γ as a function of ε and the number of degrees of freedom (n-m) are to be found in most textbooks on mathematical statistics. Such a table is given in Table A.1.

If the calculated value to be checked by the given measurement falls outside the interval defined by /III.1.4/, we decide for H_1 i.e. for the disagreement, otherwise for H_o i.e. we say that the calculated value agrees with the measurement.

Frequently, $\gamma=3$ is taken in eq. /III.1.4/ as a criterion of the agreement. This corresponds to $\varepsilon = 2.7\cdot10^{-3}$ when $n \to \infty$ i.e. when t is considered to be Gaussian. As a matter of fact, it would be possible to choose for each finite (n-m) such an ε to which $\gamma = 3$ corresponds. This is, however, very unjustified and unusual in the practice of testing hypotheses. The starting point should always be a judicious choice of ε and γ should be calculated a posteriori according to eq. /III.1.3/ for the (n-m) at hand. Therefore, the "magic" $\gamma = 3$ should be resigned of when (n-m) is not sufficiently large (i.e. much less than 100).

III.2 Confidence intervals for measurements y_i

We take up now the question left open in section II.4: to how good an approximation the equality may be expected to hold in /II.4.1/? In other words: what is the maximum of $|y_i-y_i^*|$ which is not in contradiction yet with the hypothesis that $\langle y_i \rangle = f(x_i,\underline{a})$? A quantitative answer may be formulated again only in terms of confidence intervals. Since our ultimate goal is to pick up eventual sharply defective measured values, we shall give these intervals as confidence limits for y_i.

Obviously, y_i has to be compared to y_i^*, the unbiased estimate of $\langle y_i \rangle$ given by eq. /II.4.4/. The first thing is therefore to calculate the variance of difference $(y_i-y_i^*)$. Since its expectation is zero, its variance is given by

$$\langle (y_i-y_i^*)^2 \rangle = \sigma_i^2 + \sigma_i^{*2} - 2\langle (y_i-f(x_i,\underline{a}))(y_i^*-f(x_i,\underline{a})) \rangle \qquad /III.2.1/$$

where σ_i^2 and σ_i^{*2} were estimated above /see eqs. /II.4.9/ and /II.4.8/, respectively/. Now, two cases have to be distinguished: when y_i was not taken into account in the fitting /outer point/ and when it was /inner point/.

III.2.1 Outer points

Suppose that, for some reason, y_i was left out from the fitting. It is therefore independent of both y_i^* and Q_{min}. The confidence interval is determined under the assumption that H_o is true i.e. y_i has the same mean as y_i^*. Then it follows from this that the covariance in eq. /III.2.1/ vanishes. The analog of eq. /III.1.1/ is now

$$\xi = \frac{y_i - y_i^*}{\sqrt{\sigma_i^2 + \sigma_i^{*2}}} \qquad /III.2.2/$$

which is N(0,1). Substituting σ^2 for $\tilde{\sigma}^2$ in eqs. /II.4.8/ and /II.4.9/, we have the Student fraction

$$t_i = \frac{y_i - y_i^*}{\sqrt{\sigma_i^2 + \sigma_i^{*2}}} \frac{1}{\sqrt{\frac{Q_{min}}{\sigma^2(n-m)}}} = \frac{y_i - y_i^*}{\sqrt{\frac{Q_{min}}{n-m}\{\underline{\underline{W}}^{-1} + \underline{\underline{F}}\underline{\underline{M}}^{-1}\underline{\underline{F}}^T\}_{ii}}} \qquad /III.2.3/$$

with a number of degrees of freedom equal to (n-m). Using quantile γ defined by eq. /III.1.3/, we formulate the following criterion: if

$$|t_i| > \gamma, \qquad /III.2.4/$$

we decide for H_1 i.e. we say that something is wrong with the value y_i. Other-

wise, we accept it. When $|t_i|>\gamma$ occurs, this tells with a probability $(1-\varepsilon)$ that either y_i falls outside the range of validity of function $f(x_i,\underline{a})$ or y_i is the result of a defective measurement or record.

III.2.2 Inner points

Things are much more complicated when y_i is an inner point i.e. when it was taken into account in the fitting. First, the covariance in eq. /III.2.1/ does not vanish. It may be calculated using eqs. /II.4.6/ and /II.1.12/. Neglecting the bias, we may put

$$y_i^* - f(x_i,\underline{a}) = \Delta\tilde{y}_i = \{\underline{\underline{F}}\underline{\underline{M}}^{-1}\underline{\underline{F}}^T\underline{\underline{W}}\Delta\underline{y}\}_i \qquad /III.2.5/$$

which yields

$$<(y_i-f(x_i,\underline{a}))(y_i^*-f(x_i,a))> = <\Delta y_i\{\underline{\underline{F}}\underline{\underline{M}}^{-1}\underline{\underline{F}}^T\underline{\underline{W}}\Delta\underline{y}\}_i> = \qquad /III.2.6/$$

$$= \sigma^2\{\underline{\underline{F}}\underline{\underline{M}}^{-1}\underline{\underline{F}}^T\}_{ii} = \sigma_i^{*2}$$

where eqs. /II.1.3/ and /II.4.8/ were taken into account. Finally, we have from eq. /III.2.1/ that

$$<(y_i-y_i^*)^2> = \sigma_i^2 - \sigma_i^{*2}.$$

It is interesting to remark that we had $\sigma_i^2 + \sigma_i^{*2}$ for an outer point so that we obtained:

$$<(y_i-y_i^*)^2> = \sigma_i^2 \pm \sigma_i^{*2} \qquad /III.2.7/$$

where the positive sign stands for outer points while the negative sign for inner ones. This result is quite plausible. It is a common experience that all points tend to deflect the fitted curve to themselves. Therefore, the variance of the difference $(y_i-y_i^*)$ should be definitely less than the variance of y_i alone. It is surprising, however, that this deflection is so strong that the reduction is juste by σ_i^{*2} i.e. the variance of estimate y_i^*.

Using this result, a fraction analogous to /III.2.3/ may be defined for inner points:

$$t_i = \frac{y_i - y_i^*}{\sqrt{\frac{Q_{min}}{n-m}\{\underline{\underline{W}}^{-1} - \underline{\underline{F}}\underline{\underline{M}}^{-1}\underline{\underline{F}}^T\}_{ii}}} . \qquad /III.2.8/$$

Unfortunately, this is not a Student fraction because y_i and Q_{min} are not independent. On the contrary, points which sharply stand out increase Q_{min} strongly and lead to an overestimation of σ^2. Hence, t_i as defined by eq. /III.2.8/ is expected to fluctuate less than a Student fraction. This may lead to serious mistakes in practical work when not taken into account properly, expecially if (n-m) is small.

The best solution would be to leave out point y_i from the fitting. Then the formulae of section III.2.1 would be available /of course, with (n-m-1) instead of (n-m)). This is, however, impractical. It would be too time consuming to repeat the fitting as many times as we have inner points. Fortunately, a surprisingly simple formula comes to our help. Let t_i' be the Student fraction what we would get from eq. /III.2.3/ when leaving out point y_i from the fitting. Now, it is related to t_i as

$$t_i' = \frac{t_i}{\sqrt{1 - \frac{t_i^2 - 1}{n-m-1}}} \cdot \qquad /III.2.9/$$

t_i' is by definition a Student fraction with a number of degrees of freedom equal to (n-m-1). As in the previous cases, a quantile γ may be determined for it according to eq. /III.1.3/ and we have now right to use criterion /III.2.4/ for deciding the defectiveness of point y_i. /We must not forget that t_i' should be put in /III.2.4/ for t_i/.

Once having criterion $|t_i'| > \gamma$, we may, of course, formulate an equivalent criterion for t_i in case of inner points as well. Using eq. /III.2.9/ it may be shown that $|t_i'| > \gamma$ is equivalent to

$$|t_i| > \gamma' \qquad /III.2.10/$$

where

$$\gamma' = \frac{\gamma}{\sqrt{1 + \frac{\gamma^2 - 1}{n - m}}} \cdot \qquad /III.2.11/$$

The proofs of eqs. /III.2.9/ and /III.2.11/ are lengthy. They are therefore given in Appendix 1. Table A.1 gives the values of γ' as a function of ε and (n-m): they are called there as modified Student quantiles.

It is interesting to note that t_i behaves in a strange way. It is, for example, bounded. In fact, we know from /III.2.10/ that $|t_i| < \gamma'$ with probability $(1-\varepsilon)$. Let ε tend to zero. Then $\gamma \to \infty$ and $\gamma' \to \sqrt{n-m}$ as it follows from eq. /III.2.11 . Thus, we obtained that

$$|t_i| < \sqrt{n-m} \qquad /III.2.12/$$

with probability 1. Consequently, t_i has a distribution which deviates from the Student distribution. Its statistical properties are studied in Appendix 11.

When using criterion $|t'_i|>\gamma$ for finding defective points, one should take the following remark into account. In the derivation of eq. /III.2.9/, it was assumed that all points are good except eventually point i. Let us assume now that point i_o is defective. Then criterion $|t'_{i_o}|>\gamma$ is correct but the same criterion for all other $i \neq i_o$ is not. It may be simply seen that t'_i for $i \neq i_o$ will fluctuate in this case less than expected for a Student fraction. Such a case is shown in Fig. III.4. This means that this pointwise procedure will find point i_o with a good probability and it will declare the other points to be all right. This is just what we want this criterion to do.

III.3 Remarks and numerical examples

t'_i has been defined such that it is a Student-fraction. Its distribution is entirely determined by its number of degrees of freedom i.e. by (n-m). That is why neither weights w_i nor function $f(x_i,\underline{a})$ intervene in formula /III.2.9/. We may still find remarkable that t'_i depends explicitely only on t_i and not on the other t_i. This means that these fractions are closely connected to the behaviour of the individual points y_i. This is the main reason why we recommend statistics t_i or t'_i for a pointwise analysis of the measured values y_i. The statistical properties of the t_i fractions are studied in Appendix 11. It is shown there that only (n-m) out of them are linearly independent.

The first question which arises in connection with the use of test /III.2.10/ is: what to do when the test qualifies some of the y_i defective? In order to answer this, let us estimate the probability that /III.2.10/ holds for at least one point. As mentioned in Appendix 11, this is a complicated formula because of the covariances of the $(y_i-\tilde{y}_i)$ differences. Generally, their covariances are small with respect to their variances. If we neglect them, we assume these differences as independent. The probability that the unequality does not hold for a given point is $(1-\varepsilon)$. Now the probability that it does not hold for any of the points is approximately $(1-\varepsilon)^{n-m} \approx e^{-(n-m)\varepsilon}$. For example, if $\varepsilon=0.01$ and $(n-m)=100$, this is $e^{-1} = 0.37$. Thus, the probability of finding at least one point for which /III.2.10/ holds is 0.63. According to this, in 2 out of 3 such fittings, we will find at least one point on the long run for which /III.2.10/ holds i.e. which are qualified as defective points even if everything is all right with both fitting and measurement.

This means that the appearance of such t_i values might be quite normal and does not necessarily indicate a defective y_i value. It is rather a warning signal that one should look at such points whether something is wrong with them. Most punching errors or mistakes of this kind can be eliminated in this way. Such a possibility is especially useful when one has to treat a big amount of data. This test may be considered as a check for input errors. Later in this paper, we shall see other applications, too.

It is an interesting problem whether it is worth-while to automize the data rejection on the basis of criterion /III.2.10/. We do not recommend it for the following reasons.

- In case of good measurements, this would be equivalent to a truncation of the original distribution of the y_i variables, namely too large or too small values would be excluded. The question of this modified distribution would require further study. We guess only that it remains a Gaussian with a smaller σ^2. If it is so then it has to be proven that this data rejection sequence stops with a reasonable probability before all points are rejected.
- If only a couple of points are defective, they are identified by criterion /III.2.10/ with a good probability. But, if the number of bad points is relatively large, it can not be warranted that $|t_i| > \gamma'$ occurs just for the defective points as one of the examples shows later on. /The reason is that one of our basic assumption was that, with the exception of the y_i just considered, all other inner points are unbiased./

We do not go into the details of the problem whether criterion /III.2.10/ could be improved so that it permitted an automized data rejection. For the moment, the program has to stop at the computation of the t_i fractions and at performing the comparison of $|t_i|$ and γ'.

The computation of the t_i ratios is one of the additional services of program RFIT. As it was pointed out above, they are often useful for detecting defective points. This is, however, not the only possibility of their use. It is always advisable to plot t'_i as a function of x_i. This plot has to display the same picture in all cases when the data are all right and the fit is good. Figs. III.1 and III.2 illustrate this. y_i and t'_i are plotted as functions of x_i for cases 1 and 2, respectively /see Appendix 10/. In spite of that the accuracy of the two measured curves are very different, the plots of t'_i are similar: the distribution of the points shows no tendency. In these examples, the measured curves have the same shapes /both are cosines/. In Fig. III.3, where case 4 i.e. an exponential plus a background is plotted, the plot of t'_i shows the sampe picture as in the previous figures.

Any tendency can be easily recognized on the plot of t'_i. Figs. III.4 through III.6 illustrate this point. Axial distributions are sometimes distorted by a gridplate placed near the midheight of the reactor core. Such is case 5 shown in Fig. III.4 where the flux depression is about 10 %. The effect is expecially clear in the plot of t'_i. Fig. III.5 shows case 6 i.e. the same thing with a 10 times worse statistics. Here, the presence of the effect is uncertain when only y_i is plotted but the plot of t'_i displays it somewhat more distinctly.

It may be objected that the flux depression seems to be distinct in Fig. III.5 only because we know a priori that it is present and we know where to find it. Unless we have such a theoretical expectation or a more accurate measurement such as case 5, we do not expect any tendency in many practical cases. If we look at Fig. III.5 with such an eye, we must admit that it is questionable whether we will recognize the flux depression. The lesson of Fig. III.5 is that the accuracy of this measurement is in fact not quite sufficient for this. Of course, this conclusion could be reached only on the basis of the t'_i plot.

Fig. III.4 displays the flux depression quite clearly but this is not the only thing what can be seen in the t'_i plot. First, much more t'_i values are positive than negative and, second, there are very few points for which $|t'_i|>1$ while for about half of them $|t'_i|>1$ ought to hold normally. Even if there were no peak at point $x_i = 24$, tendencies like that always indicate an ill case. If the t'_i fractions do not fluctuate sufficiently, this is always connected with a too large Q_{min}. This is sure sign of that there are several defective points in the measurement. If the number of positive and negative t'_i fractions are not about the same, this indicates a bad fit i.e. a bias in the parameter estimates. Then, of course, criterion /III.2.10/ does not work reliably.

Fig. III.6 displays an other kind of tendency.This is the plot of case 10 which is an exponential plus a background but the first few points contain an additional exponential term decaying faster than the fundamental exponential. Such curves are typical in pulsed neutron measurements. Only points $x_i \geq 5$ were taken into account in the fitting. Here, the plot of t'_i indicates not only the presence of the higher harmonic but gives also a hint where its effect is negligible.

Finally, a completely ill case is shown in Fig. III.7. Unlike the other numerical examples in this paper, this is a real doubling time measurement in which the 2^{14} bit of the scaler failed. Therefore, a big number of the y_i are too low. In this case, the plots of both y_i and t'_i display the failure but in a different way. The plot of y_i alone is clearly sufficient

for finding out which points are defective. The plot of t_i' is superfluous. It is still shown in order to illustrate how criterion /III.2.10/ works in such a case. As pointed out above, it should completely fail to work. With the exception of two points, $|t_i'|<\gamma$ i.e. it does not find the defective points. Of course, the plot of t_i' shows the defectiveness of the measurement as well as the plot of y_i: the distribution of the t_i' fractions is definitely not statistical. Which points are responsible for it, this is also evident.

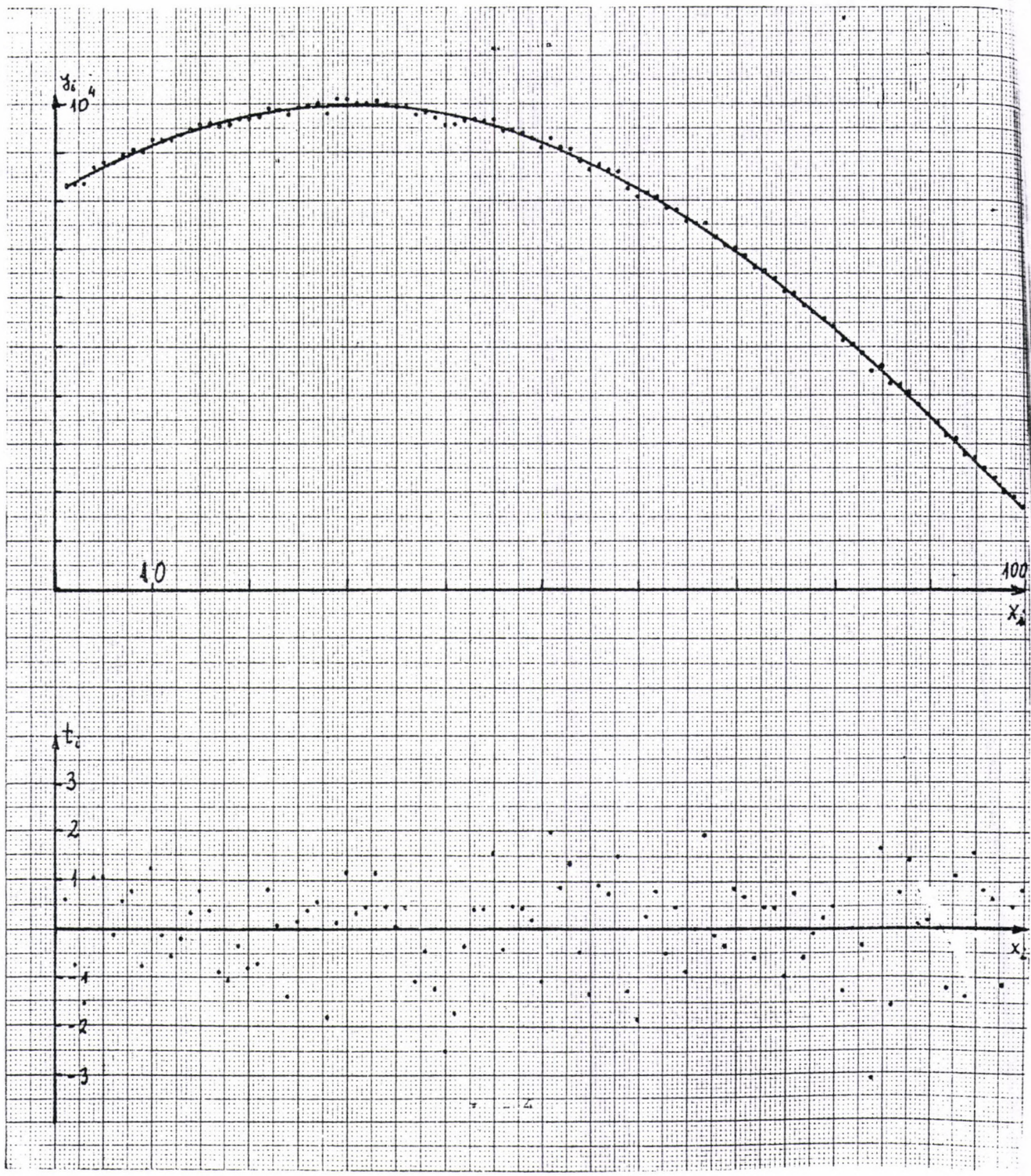

Fig. III.1

The plot of case 1

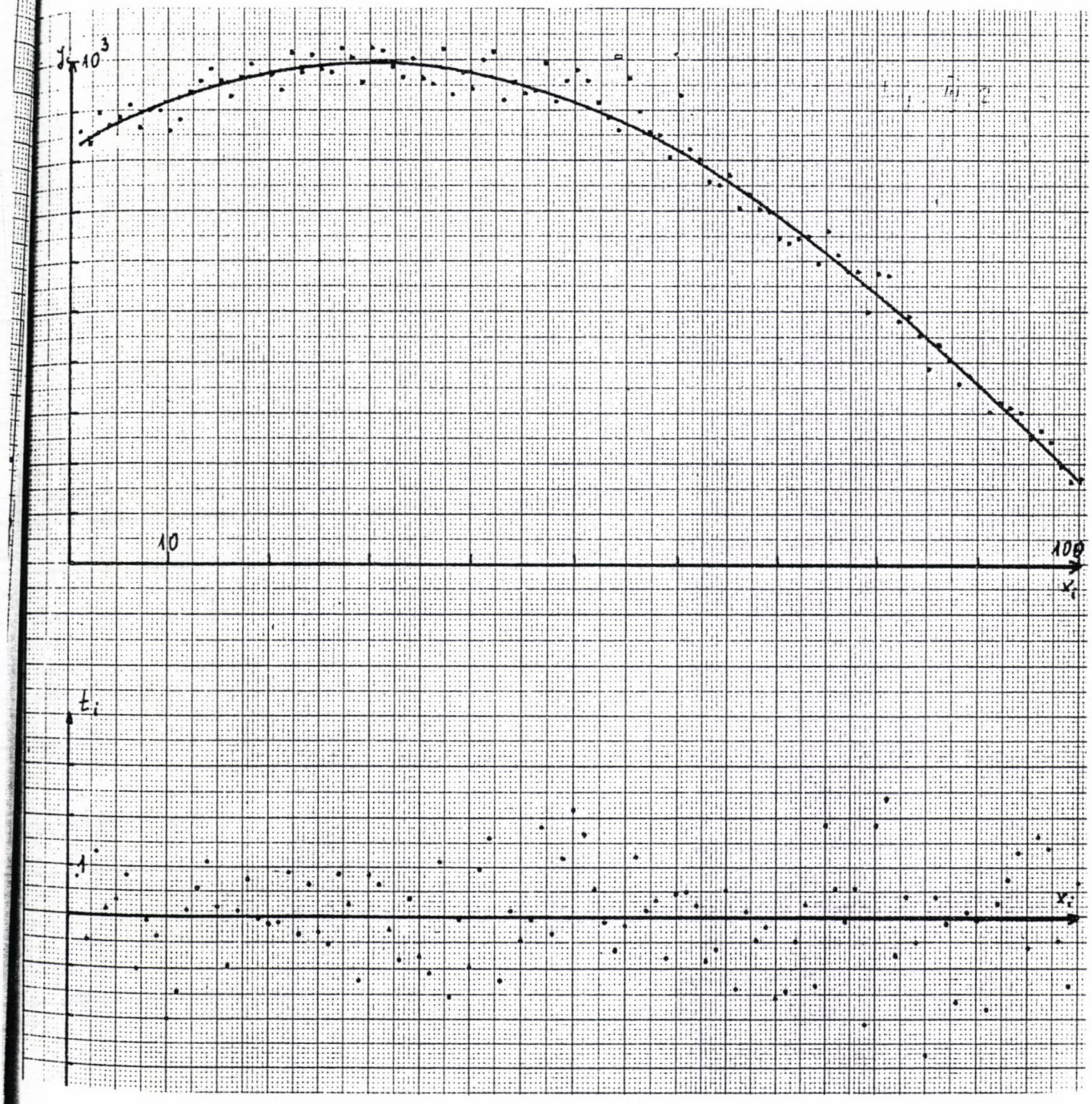

Fig. III.2
The plot of case 2

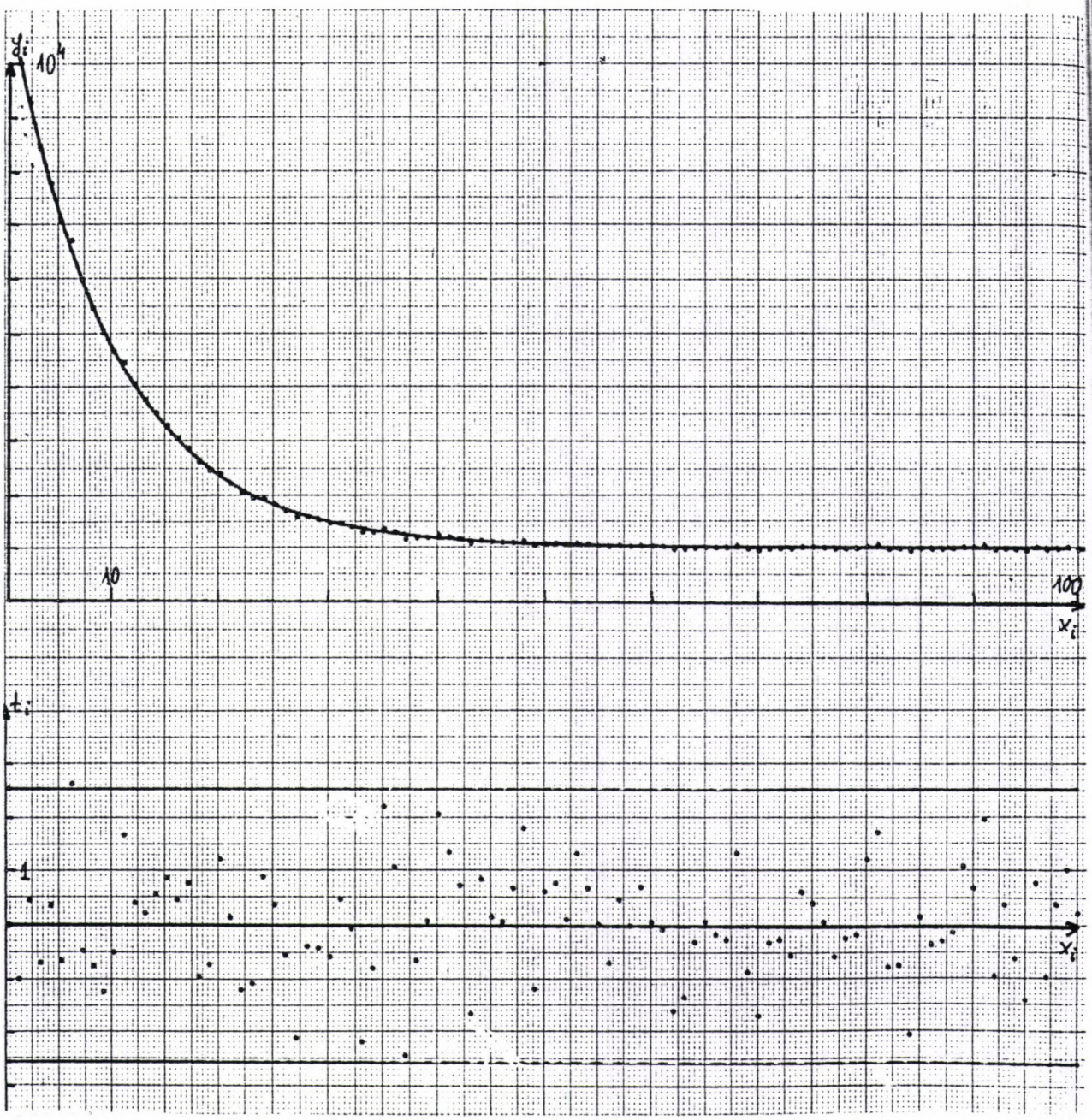

Fig. III.3

The plot of case 4

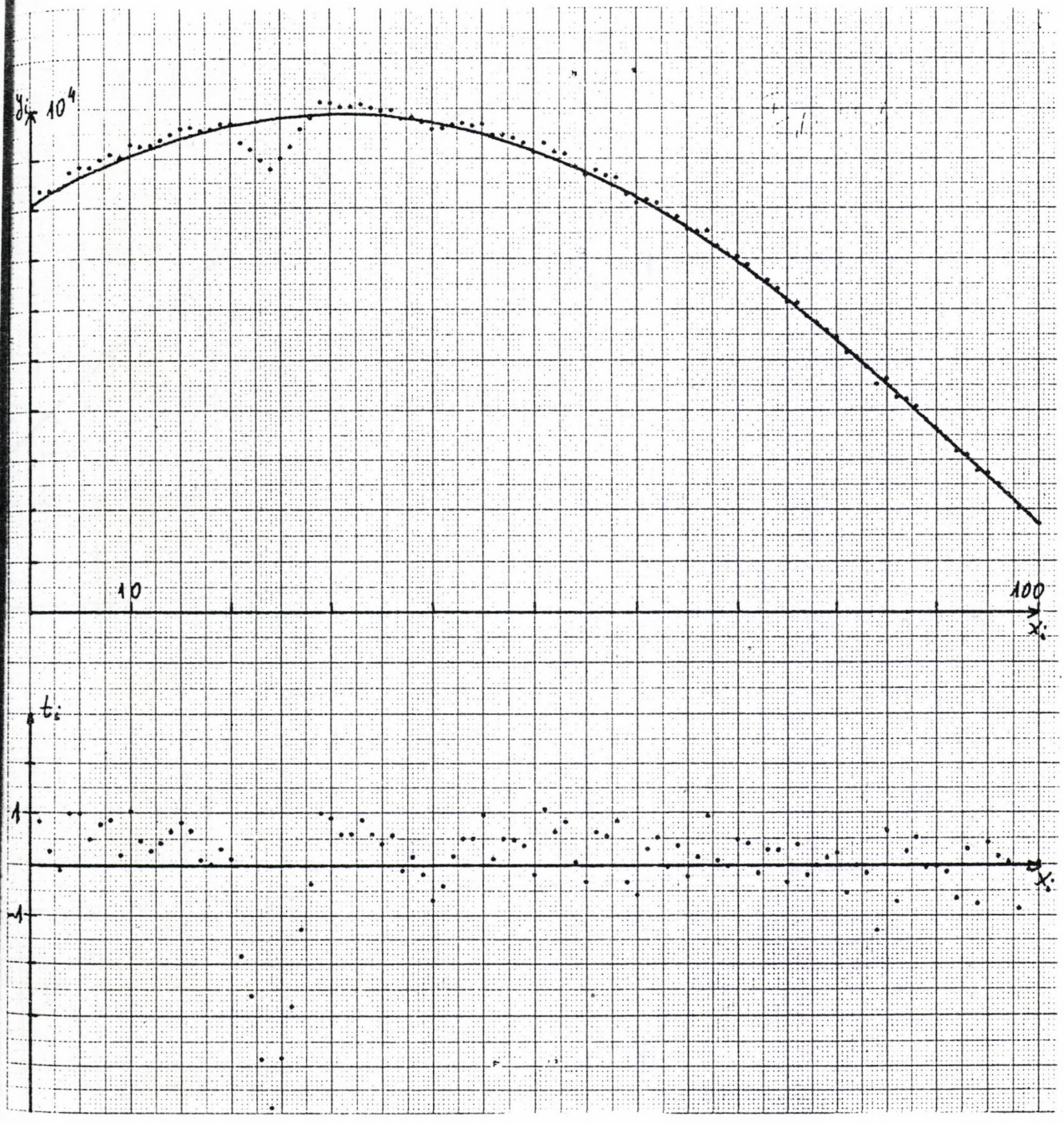

Fig. III.4

The plot of case 5

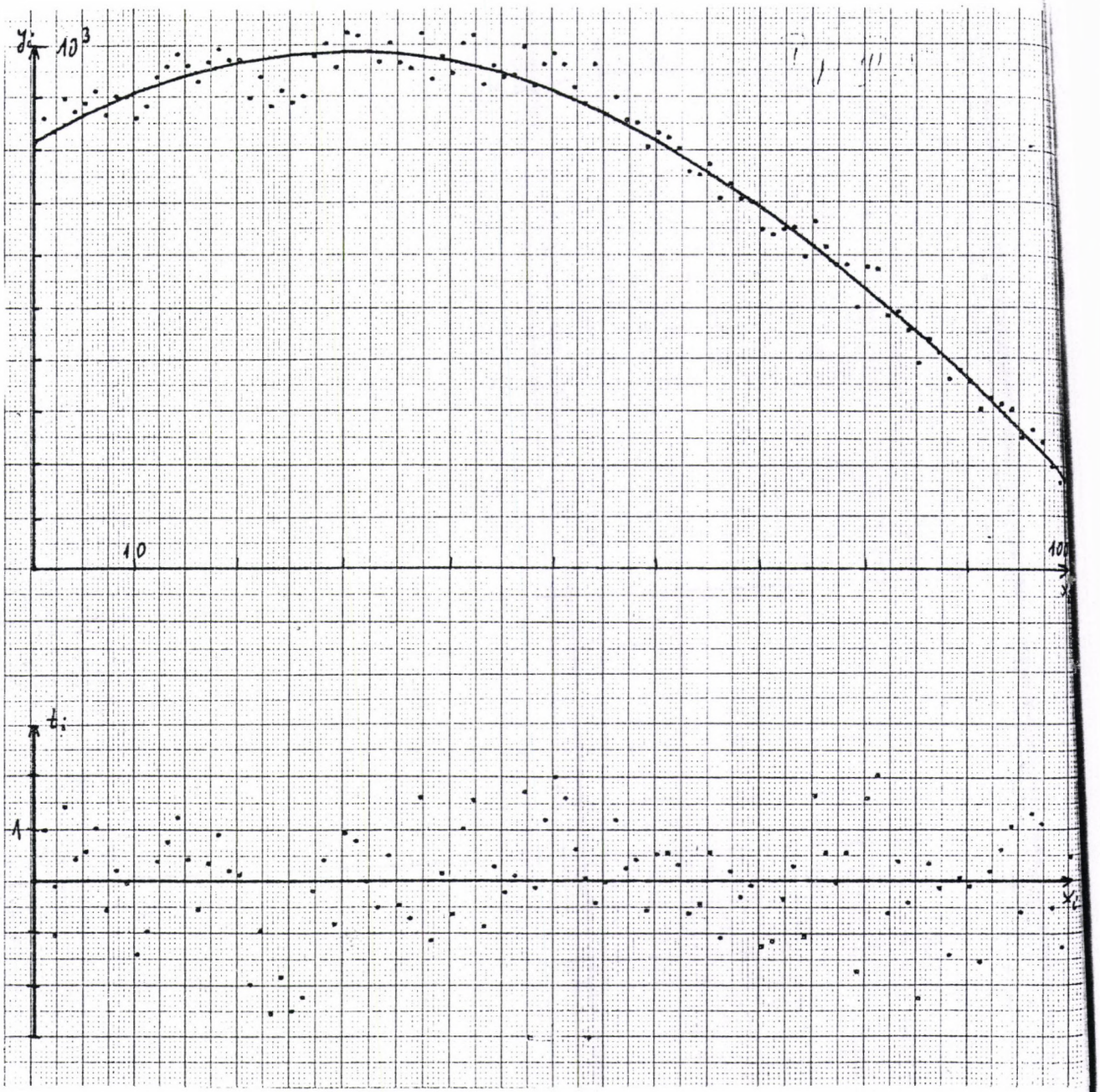

Fig. III.5

The plot of case 6

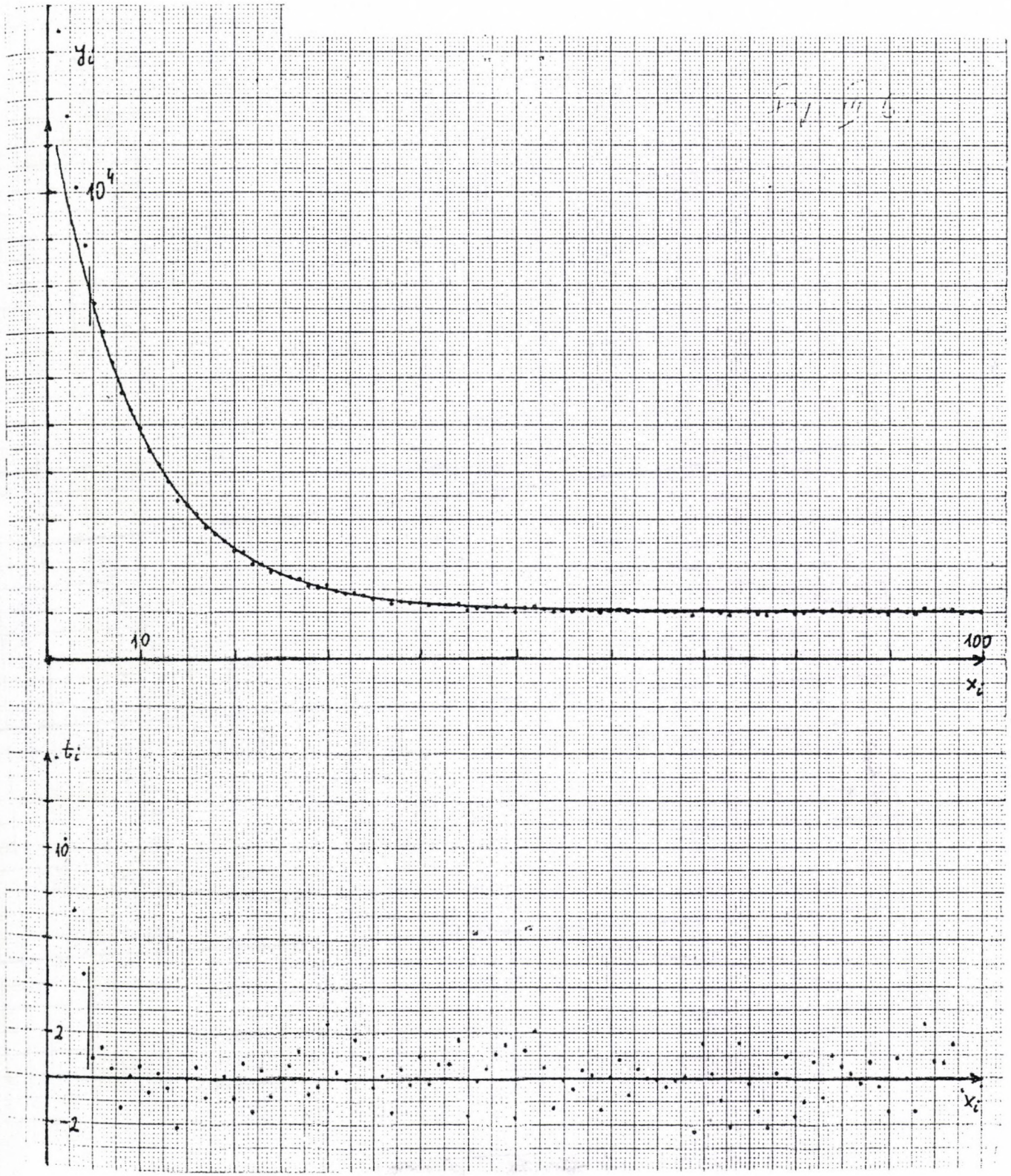

Fig. III.6

The plot of case 10

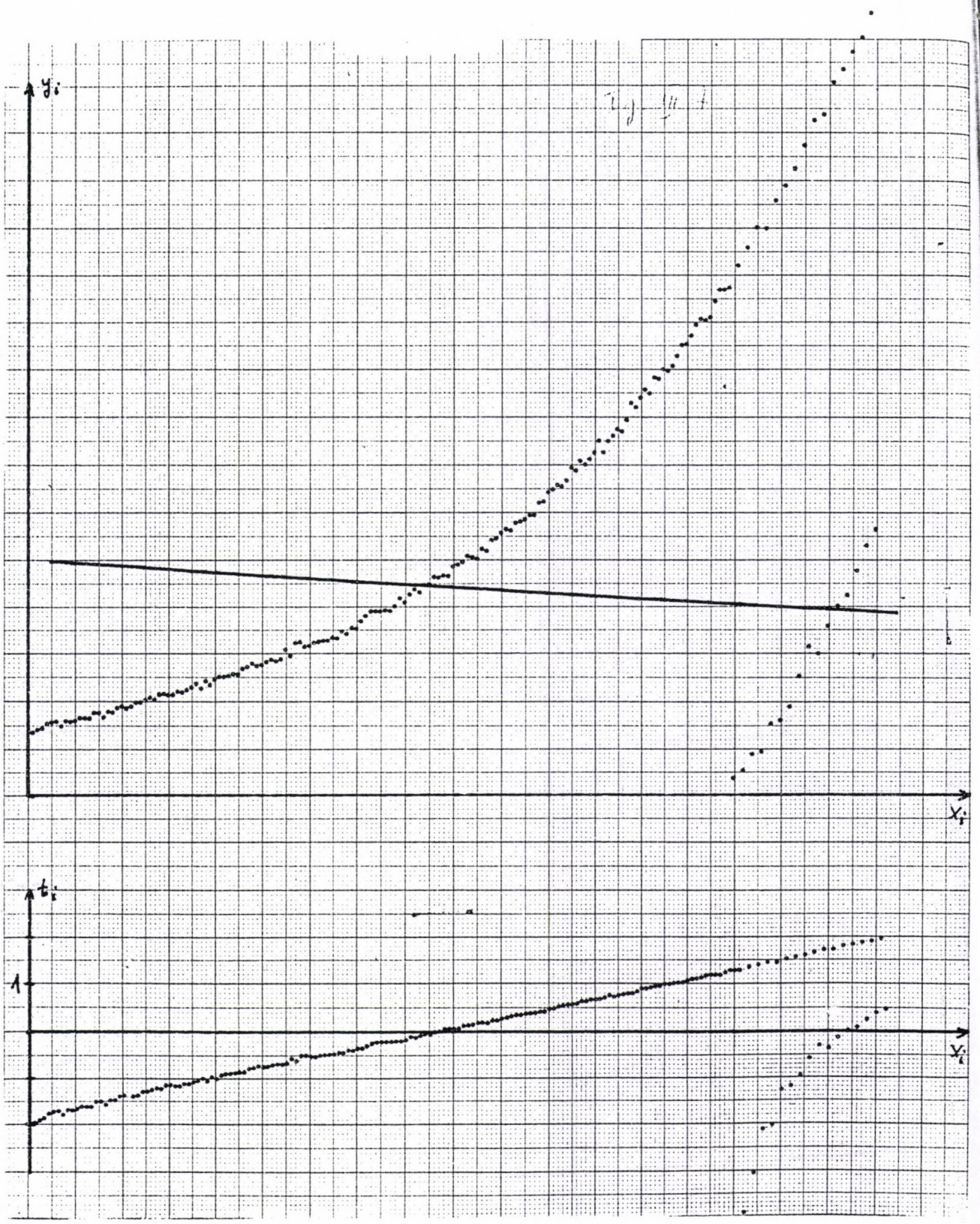

Fig. III.7

The plot of a doubling time measurement in which the 2^{14} bit of the scaler failed

CHAPTER IV.

THE POINT DROP TECHNIQUE

In reactor physics, measured curves are frequently fitted to functions $f(x_i, \underline{a})$ which are theoretically known not to satisfy eq. /I.1.2/ for all points (x_i, y_i). Those points for which eq. /I.1.2/ holds will be called asymptotic while the other ones transient. The fitting can be expected to give a reasonable parameter estimate $\tilde{\underline{a}}$ only if the transient points are deleted. Which points are asymptotic and which ones are transient, this is generally not known a priori. It is just one of the main tasks of the evaluation to tell the transient points from the asymptotic ones.

In cases when some tendencies are known from theory, the following technique came to practice in reactor physics. The "suspicious" points are dropped one by one and the fitting is repeated after each drop. If the parameter estimates show no more tendencious change when new points are dropped, we may say that we have deleted the subset of the transient points. As to when to stop dropping points, the standard textbooks of mathematical statistics give no clear cut criteria or recommendations although such criteria would be of vital importance. If too many points are dropped, we lose information unnecessarily because the standard deviations $\Delta\tilde{a}_k$ of the parameter estimates increase shaprly when points are dropped /see formula /IV.1.8//. If, in turn, not all transient points are deleted, we have to reckon with a serious bias. Thus a false decision concerning the asymptotic region influences both the bias and the standard deviation of our parameter estimates.

In the present chapter, a theory of this point drop technique is elaborated. The criteria formulated have already been introduced in the practice of reactor physics experiments and they proved to work well. This does not necessarily mean, however, that they may not be subject to improvements.

As we shall see later, both the parameter estimates and the Q_{min} values have to exhibit a behaviour controled by well defined statistical laws. The asymptotic region is characterized by constant expectation values of both parameter estimates and $\tilde{\sigma}^2$. Several criteria or statistical tests

will be derived. Which one to use in a concrete case, this depends on the actual circumstances. We shall distinguish two major cases: when σ^2 is known and when it is estimated through Q_{min}.

a/ When σ^2 is known, we may use any of two tests which are practically equivalent: the χ^2 test developed in section IV. 1 and the stepwise u-test /section IV. 3/.

b/ When σ^2 is estimated through Q_{min}, one has to check the constancy of the $\tilde{\sigma}^2$ estimates first /section IV. 2/ and only then one can test the constancy of the parameter estimates by a Fisher-test which is presented here as an improved version of the χ^2 test mentioned in a/. For this case, there exists the correspondingly modified version of the stepwise u-test of a/ which is now a stepwise Student-test.

IV.1 χ^2 test for the parameter estimates

The steps of the point drop sequence will be labelled by subscript ℓ (ℓ=1,2,...,L). In step ℓ, those points (x_i,y_i) are taken into account the subscripts of which are the elements of set I_ℓ:

$$Q_\ell = \sum_{i\in I_\ell} w_i \left[\bar{y}_i - f(x_i,\tilde{\underline{a}}_\ell)\right]^2 = \text{minimum.} \qquad /IV.1.1/$$

When some quantities defined in the previous sections get the subscript ℓ, this means that the quantity contains the contributions of only those points which belong to step ℓ. /In chapter I, the likelihood function was denoted by L. This symbol is used here for the total number of steps. In order to avoid confusion, we make the following convention: L without argument stands for the total number of steps, while with argument like $L(\underline{x},\underline{y},\underline{a})$, it stands for the likelihood function./

IV.1.1 The correlation between different steps

The behaviour of the estimates obtained in different steps can be judged only on the basis of their mutual statistical properties. As stated in section I.1, the parameter estimates are Gaussian, therefore, it is sufficient to study their variances and covariances.

The fitting yields estimate $\tilde{\underline{a}}_\ell$ in step ℓ. We calculate first the covariance matrix

$$\underline{\underline{B}}_{\ell\ell'} = \langle \Delta\underline{a}_\ell \Delta\underline{a}_{\ell'}^T \rangle \qquad /IV.1.2/$$

of estimates $\tilde{\underline{a}}_\ell$ and $\tilde{\underline{a}}_{\ell'}$, supposing that both I_ℓ and $I_{\ell'}$ contain only asymptotic points. From eq. /II.1.12/, we have that

$$\Delta \underline{a}_\ell = \underline{\underline{M}}_\ell^{-1} \underline{\underline{F}}_\ell^T \underline{\underline{W}}_\ell \Delta \underline{y}_\ell \qquad /IV.1.3/$$

where

$$\underline{\underline{M}}_\ell = \underline{\underline{F}}_\ell^T \underline{\underline{W}}_\ell \underline{\underline{F}}_\ell \qquad /IV.1.4/$$

by analogy with eq. /II.1.4/. Putting this in eq. /IV.1.2/, we get

$$\underline{\underline{B}}_{\ell\ell'} = \underline{\underline{M}}_\ell^{-1} \underline{\underline{F}}_\ell^T \underline{\underline{W}}_\ell < \Delta \underline{y}_\ell \Delta \underline{y}_{\ell'}^T > \underline{\underline{W}}_{\ell'} \underline{\underline{F}}_{\ell'} \underline{\underline{M}}_{\ell'}^{-1} .$$

Matrix $<\Delta \underline{y}_\ell \Delta \underline{y}_{\ell'}^T>$ is not necessarily a square matrix since the number of points in I_ℓ and $I_{\ell'}$ may be different. Its structure is such that its element (i,i') is $\sigma^2 \delta_{ii'}/w_i$, consequently,

$$\underline{\underline{B}}_{\ell\ell'} = \sigma^2 \underline{\underline{M}}_\ell^{-1} \underline{\underline{M}}_{\ell\ell'} \underline{\underline{M}}_{\ell'}^{-1} \qquad /IV.1.5a/$$

where element (k,k') of matrix $\underline{\underline{M}}_{\ell\ell'}$ is

$$\{\underline{\underline{M}}_{\ell\ell'}\}_{kk'} = \sum_{i \in I_\ell \cap I_{\ell'}} w_i F_{ik} F_{ik'} . \qquad /IV.1.6/$$

In an important particular case, this reduces to a simple formula. When step ℓ contains all points of step ℓ', i.e. when $I_\ell \cap I_{\ell'} = I_{\ell'}$, we may write that /cf. eq. /II.1.4//

$$\{\underline{\underline{M}}_{\ell\ell'}\}_{kk'} = \sum_{i \in I_{\ell'}} w_i F_{ik} F_{ik'} = \{\underline{\underline{F}}_\ell^T \underline{\underline{W}}_\ell \underline{\underline{F}}_{\ell'}\}_{kk'} = \{\underline{\underline{M}}_{\ell'}\}_{kk'}$$

which in eq. /IV.1.5a/ leads to

$$\underline{\underline{B}}_{\ell\ell'} = \sigma^2 \underline{\underline{M}}_\ell^{-1} \quad , \qquad \text{if } I_{\ell'} \subset I_\ell . \qquad /IV.1.5b/$$

The diagonal element (k,k) of matrix $\underline{\underline{B}}_{\ell\ell'}$ is the covariance of the estimates given for a_k in steps ℓ and ℓ':

$$<\Delta a_{k\ell} \Delta a_{k\ell'}> = \{\underline{\underline{B}}_{\ell\ell'}\}_{kk} . \qquad /IV.1.7a/$$

In the particular case when $I_{\ell'} \subset I_\ell$, we obtain from eq. /IV.1.5b/ that

$$<\Delta a_{k\ell} \Delta a_{k\ell'}> = <(\Delta a_{k\ell})^2> = (\Delta \tilde{a}_{k\ell})^2 \quad \text{if } I_{\ell'} \subset I_\ell . \qquad /IV.1.7b/$$

As a by-product of this last result, it may be shown that

$$\Delta\tilde{a}_{k\ell} \leqq \Delta\tilde{a}_{k\ell'} \quad \text{if } I_{\ell'} \subset I_{\ell}. \qquad /IV.1.8/$$

In fact, according to the Cauchy-unequality, we write that

$$<\Delta a_{k\ell}\ \Delta a_{k\ell'}> \leqq \Delta\tilde{a}_{k\ell}\ \Delta\tilde{a}_{k\ell'}\ .$$

Putting in here the covariance from eq. /IV.1.7b/, formula /IV.1.8/ is proved. This has the consequence that the standard deviation of each parameter increases monotonously when points are dropped.

In section IV.3, we shall need a generalization of the property proved in section II.5: vector $(\underline{y}_{\ell'}-\underline{\tilde{y}}_{\ell'})$ is statistically independent of $\underline{\tilde{a}}_{\ell}$ if $I_{\ell'} \subset I_{\ell}$.

By analogy with eq. /II.5.1/, we may write

$$\underline{y}_{\ell'} - \underline{\tilde{y}}_{\ell'} = \Delta\underline{y}_{\ell'} - \Delta\underline{\tilde{y}}_{\ell'} = \Delta\underline{y}_{\ell'} - \underline{\underline{F}}_{\ell'}\Delta\underline{a}_{\ell'} = \Delta\underline{y}_{\ell'} - \underline{\underline{F}}_{\ell'}\underline{\underline{M}}_{\ell}^{-1}\underline{\underline{F}}_{\ell}^{T}\underline{\underline{W}}_{\ell}\Delta\underline{y}_{\ell},$$

which combined with eq. /IV.1.3/ yields

$$<(\underline{y}_{\ell'}-\underline{\tilde{y}}_{\ell'})\Delta\underline{a}_{\ell}^{T}> = <(\Delta\underline{y}_{\ell'} - \underline{\underline{F}}_{\ell'}\underline{\underline{M}}_{\ell}^{-1}\underline{\underline{F}}_{\ell}^{T}\underline{\underline{W}}_{\ell}\Delta\underline{y}_{\ell})\Delta\underline{y}_{\ell}^{T}\underline{\underline{W}}_{\ell}\underline{\underline{F}}_{\ell}\underline{\underline{M}}_{\ell}^{-1}> =$$

$$= \sigma^2\underline{\underline{F}}_{\ell'}\underline{\underline{M}}_{\ell}^{-1} - \underline{\underline{F}}_{\ell'}\underline{\underline{B}}_{\ell\ell'} = \sigma^2\underline{\underline{F}}_{\ell'}\underline{\underline{M}}_{\ell}^{-1} - \sigma^2\underline{\underline{F}}_{\ell'}\underline{\underline{M}}_{\ell}^{-1} = 0.$$

It is noted that the same is not true for $(\underline{y}_{\ell}-\underline{\tilde{y}}_{\ell})$ and $\underline{\tilde{a}}_{\ell'}$. Only those $(y_i-\tilde{y}_i)$ are independent of $\underline{\tilde{a}}_{\ell}$, which belong to step ℓ', i.e. $i \in I_{\ell'}$. This theorem has the following corrollary:

> The Q_{min} corresponding to step ℓ' is independent of both $\underline{\tilde{a}}_{\ell}$ and $\underline{\tilde{y}}_{\ell}$ if $I_{\ell'} \subset I_{\ell}$.

IV.1.2 The constancy of a parameter

Knowing the statistical properties of estimate vectors $\underline{\tilde{a}}_{\ell}$, we now turn to the study of the behaviour of one of the fitted parameters, $\tilde{a}_{k\ell}$ $(k=1,2,\ldots,m)$. For simplicity, we denote estimates $\tilde{a}_{k\ell}$ of the chosen parameter by p_{ℓ}. By eqs. /IV.1.5a/ or /IV.1.5b/, the variance matrix $\underline{\underline{C}}$ of the p_{ℓ} is given as

$$\{\underline{\underline{C}}\}_{\ell\ell'} = <\Delta p_{\ell}\Delta p_{\ell'}> = \{\underline{\underline{B}}_{\ell\ell'}\}_{kk}\ . \qquad /IV.1.9/$$

$$\ell,\ell' = 1,2,\ldots,L$$

It is known /see e.g. [2]/ that $\underline{\underline{C}}$, being a covariance matrix, is symmetric and positive definite. As stated in section I.1, the p_ℓ may be assumed to be Gaussian. If all steps ℓ contain only asymptotic points, the expectation of p_ℓ does not depend on ℓ. This is just what we want to test and, at the same time, want to get an estimate of this common expectation value. Therefore, the following zero hypothesis H_o is formulated:

$$H_o: \qquad \langle p_\ell \rangle = p_o \qquad /IV.1.10a/$$

$$\langle \Delta p_\ell \Delta p_{\ell'} \rangle = \{\underline{\underline{C}}\}_{\ell\ell'}, \qquad /IV.1.10b/$$
$$\ell,\ell' = 1,2,\ldots,L$$

where matrix $\underline{\underline{C}}$ is defined by eq. /IV.1.9/. The alternative hypothesis H_1 is that $\langle p_\ell \rangle = p_o$ is not valid for at least one step ℓ.

Let us suppose for the time being that H_o is true. Then the probability density /i.e. the likelihood function/ of the set $p_1, p_2, \ldots, p_L$ is given by the multidimensional Gaussian distribution function:

$$L(p_1,p_2,\ldots,p_L) = \frac{1}{(2\pi)^{L/2}\left[\det \underline{\underline{C}}\right]^{1/2}} \exp\{-\tfrac{1}{2}\Gamma\} \qquad /IV.1.11/$$

with

$$\Gamma = \sum_{\ell=1}^{L} \sum_{\ell'=1}^{L} \omega_{\ell\ell'} (p_\ell - p_o)(p_{\ell'} - p_o) \qquad /IV.1.12/$$

where $\omega_{\ell\ell'}$ is an element of the inverse of matrix $\underline{\underline{C}}$:

$$\omega_{\ell\ell'} = \{\underline{\underline{C}}^{-1}\}_{\ell\ell'} \; . \qquad /IV.1.13/$$

First, the unknown p_o is estimated using the maximum likelihood principle: we choose such a value for p_o at which the likelihood function reaches its maximum. It may be seen from eq. /IV.1.11/ that this sets a minimum condition for Γ so that estimate $\tilde{p}_o$ is the solution of the equation

$$\frac{\partial \Gamma}{\partial p_o} = -2 \sum_{\ell=1}^{L} \sum_{\ell'=1}^{L} \omega_{\ell\ell'} (p_\ell - p_o) = 0. \qquad /IV.1.14/$$

We know that $\underline{\underline{C}}$ is positive definite, therefore, an extremum of Γ can be only a minimum.

It may be easily shown that

$$\tilde{p}_o = \frac{\sum_{\ell=1}^{L} \sum_{\ell'=1}^{L} \omega_{\ell\ell'} p_\ell}{\sum_{\ell=1}^{L} \sum_{\ell'=1}^{L} \omega_{\ell\ell'}} \; , \qquad /IV.1.15/$$

It is trivial now that $\tilde{p}_o$ is an unbiased estimate of p_o:

$$\langle \tilde{p}_o \rangle = p_o \qquad /IV.1.16/$$

and its variance is given by

$$\langle (\Delta \tilde{p}_o)^2 \rangle = \frac{1}{\sum_{\ell=1}^{L} \sum_{\ell'=1}^{L} \omega_{\ell\ell'}} \; . \qquad /IV.1.17/$$

Inserting $p_o = \tilde{p}_o$ in eq. /IV.1.12/, we obtain the minimum Γ_{min} of Γ. It is proved in Appendix 3 that

$$\Gamma_{min} = \chi^2_{L-1} \; . \qquad /IV.1.18/$$

This last result is just what we need: it will be the basis of testing the validity of H_o. Choose a confidence probability ε and find quantile γ_{χ^2} such that

$$P\{\chi^2_{L-1} < \gamma_{\chi^2}\} = 1-\varepsilon, \qquad /IV.1.19/$$

then H_o is accepted if

$$\Gamma_{min} < \gamma_{\chi^2} \; , \qquad /IV.1.20/$$

otherwise it is rejected in favor of H_1 /on the confidence level ε/.

<u>To summarize</u>: condition /IV.1.20/ enables us to test hypothesis H_o and, if it is found to be true, eq. /IV.1.15/ gives an estimate of the parameter in question while eq. /IV.1.17/ gives its variance.

We turn now to the particular case when

$$I_{\ell'} \subset I_{\ell} \quad \text{if} \quad \ell \leq \ell' \qquad /IV.1.21/$$

i.e. when the consecutive steps are gradually narrowing down sets I_ℓ, the broadest one being I_1. In the majority of practical cases, sets I_ℓ are chosen in that way because we know from theory that, if some I_ℓ contains only asymptotic points, so does any subset $I_{\ell'}$ of it ($\ell \leq \ell'$). In the following, we shall restrict ourselves to that case. As we have seen above, a test of H_o could be formulated in quite generality. We can go much further, however, in this particular case which - as we said already - is sufficient for most practical purposes.

From eq. /IV.1.7b/, we know that

$$\{\underline{\underline{C}}\}_{\ell\ell} = (\Delta p_\ell)^2 \; , \quad \ell \leq \ell' \qquad /IV.1.22a/$$

when /IV.1.21/ holds. This matrix has the form

$$\begin{bmatrix} (\Delta p_1)^2 & (\Delta p_1)^2 & (\Delta p_1)^2 & \ldots\ldots\ldots & (\Delta p_1)^2 \\ (\Delta p_1)^2 & (\Delta p_2)^2 & (\Delta p_2)^2 & \ldots\ldots\ldots & (\Delta p_2)^2 \\ (\Delta p_1)^2 & (\Delta p_2)^2 & (\Delta p_3)^2 & \ldots\ldots\ldots & (\Delta p_3)^2 \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ (\Delta p_1)^2 & (\Delta p_2)^2 & (\Delta p_3)^2 & \ldots\ldots\ldots & (\Delta p_L)^2 \end{bmatrix} \qquad /IV.1.22b/$$

We show that the following equations hold in this case:

$$\tilde{p}_o = p_1 \qquad /IV.1.23a/$$

$$<(\Delta\tilde{p}_o)^2> = (\Delta p_1)^2 \ . \qquad /IV.1.23b/$$

In order to prove this, we first calculate the quantities

$$\vartheta_\ell = \sum_{\ell'=1}^{L} \omega_{\ell\ell'} \ .$$

$$\ell = 1,2,\ldots,L$$

Since the $\omega_{\ell\ell'}$ are the elements of matrix $\underline{\underline{C}}^{-1}$, the ϑ_ℓ satisfy the following set of equations:

$$\sum_{\ell'=1}^{L} \{\underline{\underline{C}}\}_{\ell\ell'} \vartheta_{\ell'} = 1$$

$$\ell = 1,2,\ldots,L$$

or, inserting here the elements of $\underline{\underline{C}}$ from eqs. /IV.1.22/, this may be rewritten as

$$\sum_{\ell'=1}^{\ell-1} (\Delta p_{\ell'})^2 \vartheta_{\ell'} + (\Delta p_\ell)^2 \sum_{\ell'=\ell}^{L} \vartheta_{\ell'} = 1,$$

for $\ell = 2,3,\ldots,L$ and, for $\ell = 1$, as

$$(\Delta p_1)^2 \sum_{\ell'=1}^{L} \vartheta_{\ell'} = 1 \ .$$

It may be verified by direct substitution that the solution is

$$\vartheta_1 = \frac{1}{(\Delta p_1)^2}$$

$$\vartheta_\ell = 0$$

$$\ell = 2,3,\ldots,L$$

Thus, we obtained that

$$\sum_{\ell'=1}^{L} \omega_{\ell\ell'} = \begin{cases} \dfrac{1}{(\Delta p_1)^2} & \text{if } \ell = 1 \\ 0 & \text{otherwise} \end{cases} \qquad /IV.1.24/$$

Taking this into account in eqs. /IV.1.15/ and /IV.1.17/, we prove eqs. /IV.1.23/.

What was proved, it looks surprising at first glance. As a matter of fact, we could have foreseen it. If H_o is true i.e. I_1 contains only asymptotic points, why should we narrow it down? By dropping points from I_1, we do nothing else but merely increase the variance of our estimates /cf. formula /IV.1.8//. In other words, we throw out useful information. The further steps are used only for testing H_o but they furnish no additional information with respect to step 1. This is, in plain language, the content of eqs. /IV.1.23/. It was stated in section I.1 that the maximum likelihood estimate is efficient. We see here this general statement illustrated. We show in Appendix 4 that any other weighted average of the p_ℓ can be only a worse estimate of p_o than p_1.

Now, the question arises: what to do when H_o is found to be false? It was assumed above that sets I_ℓ are chosen such that, even if I_1 contains a few transient points, it may happen that its subset I_2 contains no more of them. Therefore, we repeat the whole procedure without taking into account step 1. If H_o is still false, we leave out step 2 as well and so on until H_o becomes true. If this does not occur at all, this means either that there is no set containing only asymptotic points or that sets I_ℓ were not properly chosen.

By this iterative procedure, we generalized the original testing procedure. We have in fact to do with a series of zero hypotheses H_o^k which may be defined as follows /cf. formula /IV.1.10//:

$$H_o^k: \quad \langle p_\ell \rangle = p_o \qquad /IV.1.25a/$$

$$\langle \Delta p_\ell \Delta p_{\ell'} \rangle = \{\underline{\underline{C}}^k\}_{\ell\ell'} \qquad /IV.1.25b/$$

$$\ell, \ell' = k, k+1, \ldots, L$$
$$k = 1, 2, \ldots, L-1$$

where $\underline{\underline{C}}^k$ is the bottom right minor of $\underline{\underline{C}}$ defined by /IV.1.22b/ containing the elements (ℓ,ℓ') for $\ell,\ell' \geq k$. $\underline{\underline{C}}^k$ is an (L-k+1) by (L-k+1) matrix. Our foregoing formulae may be simply generalized to that case. When the broadest set is I_k, the estimate for p_o is p_k with a variance equal to $(\Delta p_k)^2$ by analogy with eqs. /IV.1.23/.

The minimum of the corresponding Γ is

$$\Gamma_k = \sum_{\ell=k}^{L} \sum_{\ell'=k}^{L} \omega_{\ell\ell'}(p_\ell - p_k)(p_{\ell'} - p_k) \qquad /IV.1.26/$$

and we have instead of eq. /IV.1.18/ that

$$\Gamma_k = \chi^2_{L-k} \quad . \qquad /IV.1.27/$$

We define quantile $\gamma^k_{\chi^2}$ such that

$$P\{\chi^2_{L-k} < \gamma^k_{\chi^2}\} = 1-\varepsilon \qquad /IV.1.28/$$

and criterion for the validity of H_o^k is

$$\Gamma_k \lessdot \gamma^k_{\chi^2} \quad . \qquad /IV.1.29/$$

Appendix 5 describes a convenient algorithm for the computation of Γ_k without calculating elements $\omega_{\ell\ell'}$ of the inverse of $\underline{\underline{C}}^k$. This is so simple that it may be performed even by hand in a very short time.

In /IV.1.29/, we have a series of criteria for k=1,2,...,L-1. This leads to a series of answers. Some of them are "yes", while the others are "no". It is on the basis of these "one bit" answers that we have to decide for one of the I_k as the asymptotic region. There are at least two strategies conceivable:

- <u>strategy 1</u> or the "strategy of the first yes": all I_ℓ for $\ell \geqq k$ are considered as asymptotic if H_o^k is true but H_o^ℓ is false for all $\ell<k$. The philosophy is that, if H_o^k is true, a later "no" is considered as a mere chance.
- <u>strategy 2</u> or the "strategy of the last no": I_k is considered to be asymptotic only if H_o^ℓ is true for all $\ell \geqq k$. The philosophy is just opposite to that of strategy 1: if, after a "yes", we get a "no", the first yes is considered as a mere chance.

Both strategies are equally well justified. In practice, they seem to be almost equivalent until ε is small. On the long run, there become some differences between them sensible. These differences will be studied in section IV.4 where we shall see that the probability of false decisions strongly depends on which strategy is chosen.

The fact that the estimate for p_o is p_k in case of I_k allows the following interpretation of the generalized procedure. When analyzing steps $\ell=k,k+1,\ldots,L$, we analyse in fact the consistency of p_k with $p_{k+1}, p_{k+2},\ldots,p_L$

within the limits of the statistical accuracy. Usually, this is done when estimates p_ℓ are graphically plotted /together with the errors/ as a function of something characterizing sets I_ℓ. In most cases, almost all values agree within the statistical uncertainty although the parameter estimates clearly show some tendency for the eye: they monotonously increase or decrease. On the basis of such a plot, the best what can be done is to define the beginning of the asymptotic region at the point where the estimates begin to fluctuate. This is, however, rather subjective. Look at Fig. IV.1. On this figure, it is highly probable that point 1 is out of question. The fluctuation starts at step 4. It would be therefore orthodox to decide for step 4. More tolerant people will say that point 3 is under point 4, consequently, this is the end of the tendencious change and decide for step 3. Finally, the optimistic part of mankind will ask: if step 4 is acceptable, why not take step 2 which yielded an estimate almost equal to the estimate obtained in step 4? It is not easy to tell who is right here.

The problem was stated in a somewhat frivolous way but similar discussions frequently occur between experimentators. As to the value of the chosen parameter estimate by any of the previous decisions, there is little difference. But the standard deviations of p_2 and p_4 may differ by as much as a factor of 2! That is the point. Such a degree of subjectivity should not be allowed for. By the way, our procedure will decide for step 2 because the standard deviations increase fast from step to step. In other words, our approach is a little optimistic. The consequences of this will be studied quantitatively in section IV.4.

The fitting bias studied in section II.2 has a tendencious behaviour /see table II.2/. Its absolute value increases as points are dropped but, usually, it does not change sign. Consequently, the bias makes p_ℓ change monotonously with ℓ. This may lead to that H_o^k is found to be false for some I_k which is already asymptotic from the physical point of view. Therefore, the p_ℓ used for testing H_o^k should be corrected for bias.

IV.2 Test for Q_{min}

The procedure described in the previous section is based on the standard deviations Δp_ℓ. In each step ℓ, they are estimated by eq. /II.3.3/. Minima Q_{min} of the sums of squares are used for that purpose. This gives rise to the following problem. Until set I_ℓ contains transient points, Q_{min} will be too high and theorem /II.3.1/ will not hold. Thus, the Δp_ℓ will be also too high and the test of hypothesis H_o unrealistically too tolerant /higher standard deviations Δp_ℓ lead to smaller Γ_{min} values/. Therefore, it is necessary to study the behaviour of Q_{min} from step to step and give a

better estimate for σ^2 than eq. /II.3.2/ does. The test described in the previous section may be carried out only after this.

There is another problem with the estimation of Δp_ℓ. According to eq. /II.3.3/, Δp_ℓ depends also on matrix $\underline{\underline{M}}_\ell$ which is calculated for the parameter values obtained in step ℓ. If I_ℓ contains transient points, parameter estimate $\underline{\tilde{a}}_\ell$ may be so bad that eq. /II.3.3/ yields completely false Δp_ℓ values. It is not a rare case that even unequality /IV.1.8/ does not hold making our χ^2 test unrealistic. As it may be shown, this leads to too small values of Γ_k. Even negative Γ_k values may occur. This is another reason why we need a test in which neither σ^2 nor the parameter errors intervene.

As to the values of $Q_{min}/(n-m)$ obtained in different steps, practice shows that they are more stable than the parameter values. They become almost constant before the parameter values do. When the evaluation is carried out by hand, it is usually not a serious problem to pick up some reasonable value for σ^2. What we intend to do in this section, it is the description of a procedure which may be used in a fully automized data evaluation. We must bear in mind that decisions which are meant to be made by a computer must be formulated in a much stricter way than decisions made by man.

Let us denote the value of Q_{min} obtained in step ℓ by Q_ℓ, the number of points in I_ℓ by n_ℓ. If I_ℓ is asymptotic, we have from eq. /II.3.1/ that

$$Q_\ell = \sigma^2 \chi^2_{n_\ell - m} \quad . \qquad /IV.2.1/$$

The whole problem could be settled by saying that

$$\tilde{\sigma}^2 = \min_\ell \frac{Q_\ell}{n_\ell - m} \quad . \qquad /IV.2.2/$$

According to this, one could use the smallest one from the estimates obtained by eq. /II.3.2/ in the different steps. The philosophy behind this is that Q_ℓ is usually too high for a non-asymptotic I_ℓ. As a matter of fact, this is acceptable when no better is available. On the average of a large number of evaluations, this leads to too severe tests on one hand and to too narrow confidence intervals for the parameters on the other hand. Our main objection is, however, that it is hard to say what we should think on the statistical properties of the $\tilde{\sigma}^2$ defined by eq. /IV.2.2/. This $\tilde{\sigma}^2$, being a minimum, is surely no more distributed as $\sigma^2 \chi^2_{n_\ell - m}/(n_\ell - m)$. Its distribution is shifted to lower values. All this taken into account, we prefer the following approach.

As in the case of the parameters, we start from the statistical behaviour of the Q_ℓ. From eq. /IV.2.1/, we have that

$$\langle Q_\ell \rangle = \sigma^2 (n_\ell - m) . \qquad /IV.2.3/$$

Setting

$$Q_\ell = \sigma^2 (n_\ell - m) + q_\ell , \qquad /IV.2.4/$$

we prove in Appendix 6 that the covariance of Q_ℓ and $Q_{\ell'}$ is equal to

$$\langle q_\ell q_{\ell'} \rangle = 2\sigma^4 (n_{\ell'} - m) \qquad \text{if } I_\ell, C\ I_\ell . \qquad /IV.2.5/$$

Now as an approximation, we consider the Q_ℓ to be Gaussian with means given by eq. /IV.2.3/ and a covariance matrix given by /IV.2.5/. Under this assumption, their probability distribution is fully determined. Let us introduce the following matrix:

$$\underline{\underline{S}}^{-1} = \begin{bmatrix} (n_1-m) & (n_2-m) & (n_3-m) & \ldots\ldots & (n_L-m) \\ (n_2-m) & (n_2-m) & (n_3-m) & & (n_L-m) \\ (n_3-m) & (n_3-m) & (n_3-m) & & (n_L-m) \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ (n_L-m) & (n_L-m) & (n_L-m) & \ldots\ldots & (n_L-m) \end{bmatrix} \qquad /IV.2.6/$$

In this notation, we may write eq. /IV.2.5/ in the form

$$\langle q_\ell q_{\ell'} \rangle = 2\sigma^4 \{\underline{\underline{S}}^{-1}\}_{\ell\ell'} . \qquad /IV.2.7/$$

The matrix defined by eq. /IV.2.6/ is very similar in form to the matrix defined by eq. /IV.1.22b/. It is symmetric and positive definite if

$$n_{\ell+1} < n_\ell . \qquad /IV.2.8/$$

This condition is surely fulfilled because $I_{\ell+1} C\ I_\ell$. The likelihood function of $Q_1, Q_2, \ldots, Q_L$ is now

$$L(Q_1, Q_2, \ldots, Q_L) = \frac{(\det \underline{\underline{S}})^{1/2}}{(4\pi\sigma^4)^{L/2}} \exp\{-\frac{T}{2\sigma^4}\} \qquad /IV.2.9/$$

where T is a positive definite quadratic form:

$$T = \frac{1}{2} \sum_{\ell=1}^{L} \sum_{\ell'=1}^{L} S_{\ell\ell'} (Q_\ell - \sigma^2 (n_\ell - m))(Q_{\ell'} - \sigma^2 (n_{\ell'} - m)) . \qquad /IV.2.10/$$

$S_{\ell\ell'}$ is an element of matrix $\underline{\underline{S}}$.

According to the maximum likelihood principle, we ought to search the maximum of the likelihood function. We do not go into the details but state only that the resulting formulae are not convenient. First, the resulting estimate of σ^2 is biased. Of course, the bias vanishes in the limit when L tends to infinity /as it should according to section I.1/ but L is too small for that in practical cases. Second, a statistical test can be formulated on this basis only in a very artificial way. Therefore, we shall slightly deviate from the maximum likelihood principle and search the minimum of T defined by eq. /IV.2.10/ as a function of σ^2.

For this purpose, T is transformed as

$$T = \frac{1}{2}\left[\sum_{\ell=1}^{L}\sum_{\ell'=1}^{L} S_{\ell\ell'}Q_\ell Q_{\ell'} - \frac{Q_1^2}{n_1-m}\right] + \frac{1}{2(n_1-m)}\left[Q_1-\sigma^2(n_1-m)\right]^2 \quad /IV.2.10a/$$

The derivation of this formula is straightforward if one takes into account that

$$\sum_{\ell'=1}^{L} S_{\ell\ell'}(n_{\ell'}-m) = \begin{cases} 1 & \text{if } \ell = 1, \\ 0 & \text{otherwise.} \end{cases} \quad /IV.2.11/$$

The proof of this identity follows from that, according to eq. /IV.2.6/ this sum is an element of $\underline{\underline{S}}^{-1}\cdot\underline{\underline{S}}$. T reaches its minimum value

$$T_{min} = \frac{1}{2}\left[\sum_{\ell=1}^{L}\sum_{\ell'=1}^{L} S_{\ell\ell'}Q_\ell Q_{\ell'} - \frac{Q_1^2}{n_1-m}\right] \quad /IV.2.12/$$

when

$$\tilde{\sigma}^2 = \frac{Q_1}{n_1-m} . \quad /IV.2.13/$$

This estimate is unbiased according to eq. /IV.2.3/. Thus, we obtained that, if I_1 is asymptotic, the original estimate /given by eq. /II.3.2// may be used.

Putting Q_ℓ in eq. /IV.2.12/ from eq. /IV.2.4/, it may be simply shown that

$$T_{min} = \frac{1}{2}\left[\sum_{\ell=1}^{L}\sum_{\ell'=1}^{L} S_{\ell\ell'}q_\ell q_{\ell'} - \frac{q_1^2}{n_1-m}\right] . \quad /IV.2.14/$$

It is proved in Appendix 7 that

$$T_{min} = \sigma^4 \chi^2_{L-1} \quad /IV.2.15/$$

and Q_1 is independent of T_{min}. This is already suitable to be the basis of a statistical test.

Before formulating the test itself, the foregoing results have to be generalized to the case when only steps $\ell \geq k$ are taken into account. A similar generalization was done in section IV.1.2. We get for σ^2

$$\tilde{\sigma}_k^2 = \frac{Q_k}{n_k - m} \qquad /IV.2.16/$$

and the minimum of the corresponding T is

$$T_k = \frac{1}{2}\left[\sum_{\ell=k}^{L} \sum_{\ell'=k}^{L} S^k_{\ell\ell'} Q_\ell Q_{\ell'} - \frac{Q_k^2}{n_k - m}\right] \qquad /IV.2.17/$$

the statistical behaviour of which is determined by

$$T_k = \sigma^4 \chi^2_{L-k} \qquad /IV.2.18/$$

and T_k and Q_k are independent /see Appendix 7/. In eq. /IV.2.17/, $S^k_{\ell\ell'}$ is an element of the inverse of the bottom right minor of the matrix given in eq. /IV.2.6/:

$$(\underline{S}^k)^{-1} = \begin{bmatrix} (n_k - m) & (n_{k+1} - m) & \cdots & (n_L - m) \\ (n_{k+1} - m) & (n_{k+1} - m) & \cdots & (n_L - m) \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ (n_L - m) & (n_L - m) & \cdots & (n_L - m) \end{bmatrix} \qquad /IV.2.6a/$$

Now, the idea of testing the hypothesis that Q_k may be considered asymptotic is similar to Fisher's well known f-test /see ref. [2]/. Actually, we have two possibilities of estimating σ^2: one is given by eq. /IV.2.16/ while the other one may be obtained from eq. /IV.2.18/: $\sqrt{T_k/(L-k)}$. Now, the ratio

$$\varphi_{n_k - m, L-k} = \frac{\sqrt{T_k/(L-k)}}{Q_k/(n_k - m)} = \frac{\chi_{L-k}/\sqrt{L-k}}{\chi^2_{n_k - m}/(n_k - m)} \qquad /IV.2.19/$$

is analogous to Fisher's f-ratio which is defined as

$$f_{m,n} = \frac{\chi^2_m/m}{\chi^2_n/n} \,. \qquad /IV.2.20/$$

The only difference is the square root in the numerator of φ. We formulate now the following test: if

$$\varphi_{n_k-m,\ L-k} > \gamma_\varphi \quad , \qquad /IV.2.21/$$

$\tilde{\sigma}_k^2$ is rejected, otherwise it is accepted. γ_φ is the quantile of the distribution of φ defined as

$$P\{\varphi_{n_k-m,\ L-k} < \gamma_\varphi\} = 1-\varepsilon \ . \qquad /IV.2.22/$$

We shall refer to this test as the φ-test. Appendix 2 treats the distribution of φ and gives a table of its quantiles.

Our approach may now be summarized as follows. We carry out test /IV.2.21/ for all steps k. Here, we accept the strategy of the first yes. Let us assume that the first yes is obtained in step k*. Parameter estimate $\tilde{\underline{a}}_{k*}$ is then considered sufficiently realistic for error estimation and matrices $\underline{\underline{M}}_\ell$ are recalculated for $\ell = 1,2, \ldots, L$ with $\tilde{\underline{a}}_{k*}$ substituted for $\underline{a}$ in eq. /IV.1.4/. This in eq. /II.3.3/ together with Q_{k*} gives the errors Δp_ℓ to be used in the χ^2 test described in the previous section.

This approach is acceptable only when $(n_\ell - m)$ is sufficiently large for all steps because the χ^2 test does not take into account that Q_k* is a random variable. For small $(n_\ell - m)$, more refined methods must be used. This is the subject of the next section.

It is possible that test /IV.2.21/ does not lead to a yes for any of steps k. Then one can not do anything else than estimate σ^2 according to eq. /IV.2.2/. As a matter of fact, if this occurs, one had better to study the measured data or the definition of steps I_ℓ and find out what is wrong with them.

IV.3 Improved parameter test and confidence intervals

We supposed in section IV.1 that the standard deviations Δp_ℓ of the parameters are known. In fact, we have only estimates for them which are themselves random variables. If we do not take this into account, the χ^2 test may be misleading. This manifests itself especially when the number of degrees of freedom $(n_\ell - m)$ is small. We must, therefore, improve the approach described in section IV.1.2.

Since the trouble comes about because of σ^2, we separate it from $\underline{\underline{C}}^k$ /see eq. /IV.1.25// by setting

$$\underline{\underline{C}}^k = \sigma^2 (\underline{\underline{\Omega}}^k)^{-1} \ . \qquad /IV.3.1/$$

We denote the elements of $\underline{\underline{\Omega}}^k$ by $\omega^k_{\ell\ell'}$. The elements of $(\underline{\underline{C}}^k)^{-1}$ were denoted by $\omega_{\ell\ell'}$ in section IV.1.2. Inversion of both sides of eq. /IV.3.1/ yields that

$$\underline{\underline{\Omega}}^k = \sigma^2 (\underline{\underline{C}}^k)^{-1} \quad ,$$

consequently,

$$\omega^k_{\ell\ell'} = \sigma^2 \omega_{\ell\ell'} \quad . \qquad /IV.3.2/$$

If we put $\omega^k_{\ell\ell'}$ in eq. /IV.1.26/ for $\omega_{\ell\ell'}$, then we obtain

$$\Gamma'_k = \sum_{\ell=k}^{L} \sum_{\ell'=k}^{L} \omega_{\ell\ell'} (p_\ell - p_k)(p_{\ell'} - p_k) \qquad /IV.3.3/$$

which is related to Γ_k as

$$\Gamma'_k = \sigma^2 \Gamma_k \quad . \qquad /IV.3.4/$$

Taking into account eq. /IV.1.27/, we get that

$$\Gamma'_k = \sigma^2 \chi^2_{L-k} \quad . \qquad /IV.3.5/$$

At the stage of carrying out the test with Γ_k, we have already an estimate $\tilde{\sigma}^2$ for σ^2 obtained by the techniques described in section IV.2. This is one of the values $Q_k/(n_k - m)$. Let us denote by k^* that value of k which is favoured by our φ-test or by some other consideration. This assures that

$$\tilde{\sigma}^2_{k^*} = \frac{Q_{k^*}}{n_{k^*} - m} = \sigma^2 \frac{\chi^2_{n_{k^*}-m}}{n_{k^*}-m} \quad . \qquad /IV.3.6/$$

If we stick to the χ^2 test, we must devide Γ'_k by $\tilde{\sigma}^2_{k^*}$. Then we obtain

$$\Gamma^*_k = \frac{\Gamma'_k}{\tilde{\sigma}^2_{k^*}} = \frac{\chi^2_{L-k}}{\chi^2_{n_{k^*}-m}/(n_{k^*}-m)} \qquad /IV.3.7/$$

which is χ^2_{L-k} only in the limit when $(n_{k^*}-m)$ tends to infinity. If Γ'_k and φ_{k^*} are independent, then, for finite $(n_{k^*}-m)$, the distribution of Γ^*_k is related to Fisher's f-distribution as

$$\Gamma^*_k = (L-k)\, f_{L-k,\, n_{k^*}-m} \qquad /IV.3.8/$$

where Fischer's f-ratio was defined by eq. /IV.2.20/. Consequently, we have to modify test /IV.1.29/ to the following. We accept H^k_o if

$$\Gamma_k^* < (L-k)\gamma_f \qquad /IV.3.9/$$

and reject it otherwise. γ_f is the quantile of Fisher's f-distribution:

$$P\{f_{L-k,\ n_{k^*}-m} < \gamma_f\} = 1 - \varepsilon\ , \qquad /IV.3.10/$$

Table IV.1 illustrates the importance of this improvement for $\varepsilon = 0.05$. The row $(n_{k^*}-m)\to\infty$ corresponds to test /IV.1.29/. It may be seen from the table that, as expected, the improvement is significant when $(n_{k^*}-m)$ is small. Above about 100, there is little difference between tests /IV.1.29/ and /IV.3.9/. Cases when $(n_{k^*}-m)$ is small, occur sometimes in practice. Especially in such cases, it is important to be aware of this. The Fisher quantiles are given in Table A.2.

In formulating /IV.3.8/ and /IV.3.9/, it was assumed that Γ_k' and Q_{k^*} are independent. It was proved at the end of section IV.1.1 that $\tilde{a}_\ell$ is independent of Q_ℓ, if $\ell \leq \ell'$. Now, Γ_k' depends on all p_ℓ for $\ell \geq k$. Therefore, Γ_k' and Q_k are independent only for $k^* = L$. Thus, we conclude that only Q_L may be used for test /IV.3.9/ instead of Q_{k^*}. It follows from this that one must be careful when defining set I_L in order to have a sufficient number of points in it.

Table IV.1

Confidence limits for Γ_k' when $\varepsilon = 0.05$

$n_{k^*}-m$ \ L-k	1	2	5	10	20
10	4.96	8.20	16.65	29.1	55.4
20	4.35	6.98	13.55	22.8	42.4
40	4.08	6.46	12.25	20.0	36.8
60	4.00	6.30	11.85	19.2	35.0
100	3.94	6.18	11.50	18.5	33.6
∞	3.84	5.98	11.05	17.5	31.4

The fact that only $k^* = L$ is correct for the parameter test does not mean that the k^* picked up by the φ-test may not be used for other purposes. Let us reconsider the confidence intervals defined in chapter III.

a/ Parameters. Formula /III.1.4/ defines a confidence interval for one of the estimated parameters. This remains, of course, valid but we give here a recipe for the error estimation in the different steps. In steps $\ell \leq k^*$, Q_{k^*} is to be used for error estimation in eq. /II.3.3/ and the number of degrees of freedom is equal to $(n_{k^*}-m)$. In steps $\ell \geq k^*$, we know from the φ-test that Q_ℓ is as good as Q_{k^*}, therefore, Q_ℓ should be used in /II.3.3/ and the number of degrees of freedom is equal to $(n_\ell-m)$ i.e. formulae of section III.1 remain unchanged.

b/ Pointwise Student-test. Strictly speaking, the pointwise Student test is not possible for steps before step k^*. The reason is that although t_i can be computed for all inner points /"inner" from the point of view of step k^*/ using Q_{k^*} instead of Q_{min} in eq. /III.2.8/, the whole theory leading to the formulation of the Student test and to eq. /III.2.9/ will not be valid because of the presence of transient points. Consequently, the Student test is possible only for steps $\ell \geq k^*$. Then, of course, in the form as formulated in chapter III. As a matter of fact, we may not expect that a fitting taking yet into account transient points will detect defective points in the asymptotic region.

IV.4 The error of second kind

In the previous section, statistical tests were formulated for finding the limits of the asymptotic region. They are powerful tools if they are used in the proper way. Otherwise, they may be misleading. Therefore, in the present section, we study the probabilities and consequences of false decisions. This will help us in choosing the proper value of ε. We shall content ourselves with the analysis of the basic χ^2 test described in section IV.1.

When applying test /IV.1.29/, the probability of rejecting H_o^k is ε if H_o^k is true. Such a false rejection of the zero hypothesis is called the error of first kind. As said before, it happens with a probability of ε. If H_o^k is rejected, we turn to testing H_o^{k+1}. If it is accepted, we decide for p_{k+1}. Standard deviation Δp_{k+1} is greater than Δp_k. It follows from this that, on the long run, the error of first kind tends to increase the standard deviation of the finally accepted parameter value. In order to minimize this effect, we have an interest to choose as small a value for ε as possible.

There is, however, another point of view, too. When ε decreases, all $\gamma^k_{\chi^2}$ defined by eq. /IV.1.28/ increase and the probability of accepting false p_k values also increases. The acceptance of H_o^k when it is false is called the error of second kind. The probability of this error depends on two things: the value of ε and the deviation of the expectation values $\langle p_\ell \rangle$ from p_o.

There are many ways in which some of the $\langle p_\ell \rangle$ can differ from p_o. In order to get an insight into the behaviour and the consequences of the error of second kind, we study the following case: H_o^k is false but all of $H_o^{k+1}, \ldots, H_o^L$ are true i.e.

$$\langle p_\ell \rangle = p_o \qquad \text{for} \quad \ell = k+1, \ldots, L$$
$$\langle p_k \rangle = p_o' \neq p_o \qquad \text{/IV.4.1/}$$

Generally, it is sufficient to consider this alternative hypothesis. When several $\langle p_\ell \rangle$ are different from p_o, the resulting Γ_k values are so large that they are rejected for most typical values of ε. Therefore, only the rejection of the last false p_k is problematic. This case is formulated in /IV.4.1/.

If we use the notations of Appendix 5,

$$\Gamma_k = \sum_{\ell=k}^{L-1} \xi_\ell^2 = \Gamma_{k+1} + \xi_k^2 \qquad /IV.4.2/$$

where ξ_ℓ is defined by eq. /A.5.11/. We know that the ξ_ℓ are independent. Since $H_o^{k+1},\ldots,H_o^L$ are true,

$$\left.\begin{aligned} \langle \xi_\ell \rangle &= 0 \\ \langle \xi_\ell^2 \rangle &= 1 \end{aligned}\right\} \ell \geq k+1 \qquad /IV.4.3/$$

but, according to eq. /IV.4.1/,

$$\left.\begin{aligned} \langle \xi_k \rangle &= \frac{p_o - p_o'}{\sqrt{(\Delta p_{k+1})^2 - (\Delta p_k)^2}} = \alpha \\ \langle \xi_k \rangle &= 1. \end{aligned}\right\} \qquad /IV.4.4/$$

We ask now the probability of accepting H_o^k, i.e. $P\{\Gamma_k < \gamma^k_{\chi^2}\}$.

Since Γ_{k+1} and ξ_k are independent, this is simply given by

$$E(\alpha,\varepsilon) = P\{\Gamma_k < \gamma^k_{\chi^2}\} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{(x-\alpha)^2}{2}} P\{\Gamma_{k+1} < \gamma^k_{\chi^2} - x^2\}dx. \qquad /IV.4.5/$$

H_o^{k+1} being true, the distribution of Γ_{k+1} is the distribution of χ^2_{L-k-1}, consequently, the integral may be calculated in a straightforward way. /When (L-k) is odd, explicite analytical expressions may be obtained while we must integrate numerically for an even (L-k)./

Usually, $1-E(\alpha,\varepsilon)$ is called the <u>power</u> of the test. It is the probability of rejecting H_o^k. For $\alpha = 0$, it is by definition equal to ε i.e.

$$1 - E(0,\varepsilon) = \varepsilon \qquad /IV.4.6/$$

while it tends to 1 as α increases. In fact, it is the behaviour of the power function what tells a good test from a poor one. The larger it is for a given α, the better the test is.

The quantity of interest for us is $\alpha E(\alpha,\varepsilon)$. Let us suppose that both measurement and evaluation are repeated N times. The expected number of cases when H_o^k will be accepted is $NE(\alpha,\varepsilon)$. Then the expectation of the average of the parameter values favoured by the test will be equal to

$$\frac{p'_o NE(\alpha,\varepsilon) + p_o[N-NE(\alpha,\varepsilon)]}{N} = p_o + (p'_o-p_o)E(\alpha,\varepsilon) =$$

$$= p_o - \alpha E(\alpha,\varepsilon)\sqrt{(\Delta p_{k+1})^2 - (\Delta p_k)^2} \ . \qquad /IV.4.7/$$

This shows that we have a systematic error, i.e. a bias which is proportional to $\alpha E(\alpha,\varepsilon)$.

As an illustration, Fig. IV.2 shows $\alpha E(\alpha,\varepsilon)$ as a function of α for L-k=6 and ε=0.01, 0.05 and 0.1. For all other values of ε and (L-k), the corresponding curves are similar*. For both small and large values of α, $\alpha E(\alpha,\varepsilon)$ is small. This is explained by that large α values are accepted with a vanishingly small probability while small α values are although accepted with a relatively large probability /approximately$(1-\varepsilon)$/ but they result in a small change with respect to p_o. The curve $\alpha E(\alpha,\varepsilon)$ vs. α exhibits a maximum. This is at the most dangerous value of α: it is high enough for leading to a large bias but it is still accepted with a not too small probability. In the following, we shall use this maximum value as an upper bound of the bias caused by the error of second kind.

This bias appears for the strategy of the first yes /see section IV.1/ as it was obtained above but it is reduced by $P_{L-k}(\varepsilon)$ for the strategy of the last no where $P_{L-k}(\varepsilon)$ is the probability of accepting all of $H_o^{k+1}\ldots,H_o^L$. Consequently, the following δp_o is an upper bound of the bias

$$\delta p_o = P_{L-k}(\varepsilon)\sqrt{(\Delta p_{k+1})^2 - (\Delta p_k)^2}\ \max[\alpha E(\alpha,\varepsilon)] \qquad /IV.4.8/$$

where $P_{L-k}(\varepsilon)$=1 has to be substituted for the strategy of the first yes. Figs. IV.3 show $P_{L-k}(\varepsilon)\ \max[\alpha E(\alpha,\varepsilon)]$ as a function of ε for some values of (L-k) and for both strategies.

On the basis of this figure, the following conclusions may be drawn:

- δp_o is sharply decreasing with ε especially until ε is small (<0.05).
- Strategy 2 is definitely more favourable than strategy 1 from the point of view of δp_o.
- Large values of (L-k) are not favourable, especially in case of strategy 1. For strategy 2, this tendency changes only in the range ε>0.3 /not

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* All curves shown in Figs. IV.2 through IV.5 were calculated by F. Adorján.

shown in Fig. IV.3/. Therefore, it is not advantageous to work with too many sets I_ℓ which are asymptotic.

These conclusions may be completed by a further one on the basis of eq. /IV.4.8/. Figs. IV.3 show only $P_{L-k}(\varepsilon)\max[\alpha E(\alpha,\varepsilon)]$ but δp_o depends also on $\sqrt{(\Delta p_{k+1})^2 - (\Delta p_k)^2}$. This factor is generally near Δp_k. /It is rarely less than half or one third of Δp_k./ Therefore, δp_o is of about the same order of magnitude as Δp_k. This is an important property of δp_o. It is annoying because it entails that the systematic error due to this bias is roughly proportional to the statistical error. Consequently, the usefulness of the point drop technique is questionable in case of inaccurate measurements. But it is at the same time an advantage because it shows the ways of reducing δp_o. /We return to this point in section V.2./ Factor $\sqrt{(\Delta p_{k+1})^2 - (\Delta p_k)^2}$ can be minimized by dropping the minimum number of points in step (k+1). This is in fact an almost trivial conclusion: every experienced experimentator will drop points in very fine steps in the region where he guesses the limit of the asymptotic region. Our considerations show only the consequences of not following this simple principle. One must not forget, however, that this conclusion is valid only under assumption /IV.4.1/. In connection with Figs. IV.13, we shall see that there are cases in which the expectations $\langle p_k \rangle$ decrease so slowly that there is no step k for which /IV.4.1/ would hold. This leads to small values Γ_k also for k values for which $\langle p_k \rangle$ is far from p_o yet. The result is a large bias in the chosen parameter value. This effect can be reduced by dropping more points in the subsequent steps. Fortunately, such difficult cases are relatively rare. In the practice of the author, they were met only for exponential fitting functions /in pulsed neutron reactivity measurements./

Up to now, only the consequences of the error of second kind were studied. They could be expressed through the appearance of bias δp_o. It was shown that it can be minimized by as large an ε as possible. As mentioned above, the increase of ε leads to an increase of the statistical error due to the error of first kind. Let us denote by $P\{\ell\}$ the probability of choosing step ℓ. If p_ℓ is chosen as $\tilde{p}_o$, the variance of this $\tilde{p}_o$ is $(\Delta p_\ell)^2$, therefore, the expectation of the variance of the finally chosen $\tilde{p}_o$ is

$$\langle (\Delta \tilde{p}_o)^2 \rangle = \frac{\sum_{\ell=k}^{L} P\{\ell\}(\Delta p_\ell)^2}{\sum_{\ell=k}^{L} P\{\ell\}} \quad . \qquad /IV.4.9/$$

Before going further, it is noted that, strictly speaking, the quantity defined by eq. /IV.4.9/ is not sufficient for characterizing the consequences of the error of first kind. Namely, it may happen that none of H_o^k is found to be true. In this case, the whole fitting is rejected. This may happen even if everything is all right with both fitting and measurement.

For strategy 1, this occurs with a relatively small probability while, for strategy 2, the probability of such a situation is ε. Fig. IV.4 shows this probability i.e.

$$1 - \sum_{\ell=1}^{L} P\{\ell\}$$

as a function ε for strategy 1. For large values of ε, this effect of the error of first kind may be important but we leave it out of consideration for the time being.

Probabilities $P\{\ell\}$ are rather complicated functions of ℓ, L, and ε. They depend also on whether strategy 1 or 2 is chosen. They were therefore determined by Monte Carlo techniques.

Figs. IV.5 show $\sqrt{<(\Delta p_o)^2>}$ and δp_o vs. ε for some values of (L-k) for case 1 /see Appendix 10/ when 2 points are dropped in each subsequent step. These curves allow to make the following conclusions:

- For small values of ε /i.e. near 0.01/, bias δp_o and the statistical error are comparable for both strategies.
- The statistical error increases much slower than δp_o decreases - at least in the range $\varepsilon<0.1$. When ε further increases, δp_o decreases approximately as fast as the statistical error increases.
- Except for large values of ε, strategy 2 seems to be more advantageous than strategy 1.
- Both the statistical error and the bias increase slightly with (L-k) i.e. the number of steps after the step just considered. Nevertheless, this effect is small.

On the basis of these curves, we could recommend to choose strategy 2 and to use an ε in the range 0.05 ÷ 0.1. Of course, this must by no means be considered as a general recommendation. For each actual type of measurement, such an analysis has to be made.

A consequent use of strategy 2 would frequently lead to the rejection of the whole fitting. If, for example, $\varepsilon = 0.1$, each 10^{th} fitting will be rejected just for statistical reasons. /As Fig. IV.4 shows, about each 50^{th} case would be rejected for strategy 1./ It follows from the definition of strategy 2 that none of the steps is found asymptotic if H_o^{L-1} is false. When such cases occur frequently, most people regret the effort spent for performing the measurement of the cases to be rejected and one is rather inclined to blame strategy 2 instead of the measurement. Such a human weakness can be excused by the following argument: if step L had not been taken into account, the case could have been saved. As a conclusion, one goes over

to strategy 1. It seems now that strategy 1 with a reasonably large ε is optimal.

These considerations were too general. The philosophy of choosing ε and strategy depends on the actual circumstances and mainly on the ultimate goal of the evaluation. Sometimes, δp_o is to be minimized, sometimes the statistical error has to be as small as possible, and there may be cases when something else has to be optimized. Consequently, it may happen that, from the same set of values $p_1, p_2, \ldots, p_L$, different ones are chosen in different situations. For this reason, only parameter estimates $\tilde{a}_\ell$ and their variances may be considered as the final results of the fitting. Program RFIT performs the χ^2 or Fisher-test with a preset value of ε=0.05. This, however, is done only in order to give the program's users some first idea on their data.

IV.5 Some further approaches

In the previous sections, a possible approach was described in detail. There are, of course, other possibilities, too. A couple of them will be cited on the following pages.

IV.5.1 Physical arguments

Our approach was based purely on mathematical arguments. This makes it sometimes fragile. It is always advantageous to let also some physical arguments intervene. Therefore, the measurements are sometimes carried out in such a way that the limit separating asymptotic and transient regions became physically evident. The idea is made clear on the example of the axial flux distribution measurement.

The asymptotic distribution is characterized not only by the cosine shape but also by the constancy of the spectrum. In the transient region, the spectrum depends on poisition. Therefore, if we measure axial distributions with two detectors of different spectral sensitivities, the shapes of the activity distributions will be different in the transient region. It follows from this that the spectral indices i.e. the activity ratios of these two detectors will be constant in the asymptotic region while they will show some tendencious change /a monotonous increase or decrease/ in the transient region. It seems now that the limit of these two regions may be found by such a physical argument. This would be blameless if we knew these spectral indices exactly but this is, unfortunately, not the case. The spectral indices have also some statistical uncertainty and their constancy can be stated only by statistical methods. To put it the other way: another hypothesis test has to be formulated.

Let us denote the experimental value of the spectral index in point x_i by s_i and let its variance be

$$\langle (\Delta s_i)^2 \rangle = \frac{\sigma^2}{w_i} \quad . \qquad /IV.5.1/$$

$$i = 1, 2, \ldots, n$$

According to what was said above, we wish to test the following zero hypothesis:

$$H_o: \quad \langle s_i \rangle = s_o \qquad /IV.5.2/$$

where s_o is the /unknown/ constant value of the spectral index around which the measured spectral indices fluctuate. The present case is simpler than the case of the fitted parameters because the spectral indices s_i are independent from each other. Supposing that H_o is true, it is trivial /see e.g. eq. /II.3.1// that

$$Q = \sum_{i=1}^{n} w_i (s_i - \bar{s})^2 = \sigma^2 \chi^2_{n-1} \qquad /IV.5.3/$$

where

$$\bar{s} = \frac{\sum_{i=1}^{n} w_i s_i}{\sum_{i=1}^{n} w_i} \quad . \qquad /IV.5.4/$$

Now, we have the following possibilities:

a/ If σ^2 is known /i.e. we trust our error estimation/, eq. /IV.5.3/ offers a means of making a χ^2 test of H_o. If it turns out to be false, we drop some points and repeat the test with the reduced set of points. This is continued until H_o is found to be true. This approach is essentially the same as the one described in section IV.1.2 apart from the number of degrees of freedom.

b/ If σ^2 is not supposed to be known /what is usually the case/, eq. /IV.5.3/ may be used only for the estimation of σ^2. In this way, the problem is again reduced exactly to the case treated in the previous sections. We may carry out a point by point Student test as described in section III.2 or we may analyse the behaviour of $\bar{s}$ as points are dropped according to sections IV.1 to IV.3.

We see that spectral indices do not help more in looking for the limit of the asymptotic region than the analysis of the behaviour of the fitted parameters. As a matter of fact, they require some additional effort which does not pay anything. The point is that we must carry out the cosine fitting anyhow in order to determine the axial buckling and we will verify

whether the parameter test confirms the conclusions made on the basis of the spectral indices. To summarize: It is preferable to base the decisions on the behaviour of the parameter we are interested in and to use the spectral indices there where they contain useful additional information, namely in the transient region /e.g. for comparison with calculated distributions taking into account spectral changes in the transient region/.

IV.5.2 Stepwise Student test

It was shown in Appendix 5 that ξ_ℓ defined in eq. /A.5.11/ is N(0,1). This is true only if we know σ^2. In fact, we know only

$$\Delta p'_\ell = \frac{\Delta p_\ell}{\sigma} \qquad /IV.5.5/$$

so that only

$$u_\ell = \frac{p_{\ell+1} - p_\ell}{(\Delta p'_{\ell+1})^2 - (\Delta p'_\ell)^2} = \sigma \xi_\ell \qquad /IV.5.6/$$

may be calculated in practice. It was mentioned at the end of section IV.3 that Q_ℓ, and $\tilde{\underline{a}}_\ell$ are independent if I_ℓ, C I_ℓ. Since $I_{\ell+1}$ C I_ℓ, we conclude from this that both $p_{\ell+1}$ and p_ℓ are independent from $Q_{\ell+1}$. Therefore,

$$t_\ell = \frac{u_\ell}{\sqrt{\frac{Q_{\ell+1}}{n_{\ell+1}-m}}} = \frac{\xi_\ell}{\sqrt{\frac{\chi^2_{n\ell+1}-m}{n_{\ell+1}-m}}}$$

in a Student fraction with a number of degrees of freedom $(n_{\ell+1}-m)$.

If the φ-test qualifies step $(\ell+1)$ as non-asymptotic, it may not be assumed that $Q_{\ell+1} = \sigma^2 \chi^2_{n_{\ell+1}-m}$. In section IV.3, the first step which is found as asymptotic by the φ-test was denoted by k^*. Therefore, the proper definition of this Student fraction is

$$t_\ell = \begin{cases} \dfrac{u_\ell}{\sqrt{\frac{Q_{k^*}}{n_{k^*}-m}}} & \text{if } \ell + 1 \leq k^* \\ \dfrac{u}{\sqrt{\frac{Q_{\ell+1}}{n_{\ell+1}-m}}} & \text{if } \ell + 1 \geq k^* \end{cases} \qquad /IV.5.7/$$

This offers a means of making a stepwise Student test. If we calculate t_ℓ for $\ell=1,2,..,L-1$, the resulting values may be used in the following ways:

- The χ^2 or the Fisher test is always based on a quantity which characterizes the behaviour of the parameter estimates globally. If it is found that something is wrong globally, the study of the Student fractions shows which step/s/ is /are/ responsible for that.
- The stepwise fractions t_ℓ are analogous to the pointwise fractions t_i defined by eq. /III.2.8/. As written in chapter III, such fractions are especially useful when the significance of some tendencies is studied. The whole point drop technique was developed just to discover such tendencies. They are hardly seen when the parameter values p_ℓ are studied but they become clear from the behaviour of the t_ℓ. The next section shows a couple of examples for this.

As a matter of fact, the study of the behaviour of fractions t_ℓ may be considered as an alternative test which may substitute the Fisher test or the χ^2 test. /The latter only if $(n_{k*}-m)$ is large./ If this is done, always two subsequent steps are compared with each other. We do not go into the details of this but only remark the following without proof:

- The bias due to the error of the second kind increases fast as ℓ increases. Therefore, this test exhibits a bad behaviour from this point of view.
- The probability of the error of the first kind is definitely less for this test than for the χ^2 or the Fisher test. This means that the statistical error increases slower with ε.

We see that this stepwise Student test may be better or worse than the tests studied in the previous sections. It would be interesting to study in which cases this test is superior. In practical cases, the stepwise and the global approaches seem to be almost equivalent.

In a completely analogous way, the fractions

$$\vartheta_\ell = \frac{\frac{Q_{k+1}}{n_{k+1}-m} - \frac{Q_k}{n_k-m}}{\frac{Q_k}{n_k-m}\sqrt{\frac{2}{n_{k+1}-m} - \frac{2}{n_k-m}}} \qquad /IV.5.8/$$

defined by eq. /A.7.24/ may be used as well for making a stepwise test for studying the behaviour of the Q_ℓ values. This is an approach alternative to the φ-est. As in the case of fractions t_ℓ, the test based on them is roughly equivalent to the global φ-test described in section IV.2. Similarly to the use of the t_ℓ, they can be useful in studying some tendencies.

IV.6 Numerical examples

We finish the present chapter by some numerical examples in order to illustrate how these tests work in practice. All examples are simulated measurements specified in Appendix 10. All test are made with $\varepsilon=0.05$.

Figs. IV.6 show the results obtained for case 1 using

$$f(x,\underline{a}) = a_1 \cos[a_2(x-a_3)] \qquad /IV.6.1/$$

as the fitting function. The step intervals I_ℓ were defined in the following way: I_1 is interval /1,95/, I_2 is /1,93/ and so on until I_{20} which is interval /1,57/. The results of the fitting are plotted as functions of the largest x_i taken into account i.e. results from step 1 at x = 95, form step 2 at x = 93 etc. In Fig. IV.6a, the values of Q_ℓ are plotted. In addition to this, the limits for $\pm\sqrt{2Q_\ell/(n_\ell-m)}$ are also shown. The values of ϑ_ℓ defined by eq. /IV.5.8/ are plotted in Fig. IV.6b. The φ-test accepts step 1 as asymptotic /as it should be/. Fig. IV.6c shows the values of $\tilde{a}_2$ together with the error estimates. In Fig. IV.6d, Student fractions t_ℓ defined by eq. /IV.5.7/ are plotted for this parameter. The Fisher test, too, qualifies step 1 as asymptotic. The result from this step for a_2 is $/2.0100\pm0.0063/\cdot10^{-2}$ leading to a confidence interval $/1.993,\ 2.027/\cdot10^{-2}$ for $\varepsilon=0.01$ which contains the true value 0.02. Case 1 is shown only in order to illustrate how these quantities behave in a theoretically pure case. The next examples will already contain really transient points.

Figs. IV.7 show the results for case 7. The fitting function was chosen again according eq. /IV.6.1/. Figures a,b,c,d show the same quantities as explained above for case 1. Case 7 is typical for a fairly accurate measurement. The tendencies due to the appearance of transient points in the first few steps are very well seen from the behaviour of both t_ℓ and ϑ_ℓ. The step favoured by both the φ- and Fisher tests is step 9 for which $\tilde{a}_2 = (1.979\pm0.011)\cdot10^{-2}$ leading to the following confidence interval $(1.950,\ 2.008)\cdot10^{-2}$ for $\varepsilon=0.01$. According to the theory outlined in section IV.4, the upper bound for the systematic error /i.e. δp_o in the notations of section IV.4/ is $6.5\cdot10^{-5}$ which is about 0.3 % of the true a_2 value. We know from the tendencies observed in Fig. IV.7 that the systematic error is negative. It would not be proper, however, to add this value to $\tilde{a}_2$ as a correction because this δp_o is only an upper bound and not an estimate in the sense of mathematical statistics. As to Fig. IV.7c, it is noted that the standard deviations indicated are not the proper ones. They are the estimates for $\Delta\tilde{a}_2$ obtained in the individual steps i.e. not recalculated with the parameter estimates obtained in step 9. As the figure shows, these estimates are so bad that they even decrease in the first few steps while they ought

to increase according to formula /IV.1.8/. This illustrates the importance of our conclusion that the standard deviations should always be recalculated for the parameter values obtained from the step favoured by the φ-test.

It is interesting to verify our choice of the limit of the asymptotic region in the direct plot of the y_i values. Fig. IV.8 shows this plot together with the pointwise fractions t'_i introduced in section III.2. Our tests qualified step 9 as asymptotic i.e. points $x_i \leq 79$ are all asymptotic at this confidence level. This limit is marked in Fig. IV.8. It seems to be a good choice visually. We must not think, however, that we could have chosen this limit visually in such a succesful way. The fact is that, for a real experiment, we can plot only y_i vs. x_i without the fitted /continuous/ curve. Now, if we do not consider the fitted curve, we would probably choose point $x_i=85$ as the limit of the asymptotic region. This is our step 6 for which the estimate is $\tilde{a}_2=(1.933\pm0.009)\cdot10^{-2}$ leading to a systematic error of about 3.5 %. This warns that one must not rely on visual decisions. We remark finally that pointwise fractions t_i and stepwise fraction t_ℓ show the tendencies in the transient region practically in the same way /see Table IV.2/.

Figs. IV.9 and IV.10 show the analogous results for case 8. This is the same as case 7 but the statistics is 10 times poorer. Comparison of Figs. IV.9 and IV.7 shows that the same tendencies are much less to be seen although the shape of the $\langle y_i \rangle$ vs. x_i curves are identical. The φ-test chooses step 7 while the Fisher test step 8 for which $\tilde{a}_2=(2.011\pm0.031)\cdot10^{-2}$. The corresponding asymptotic region is $x_i \leq 81$ as indicated in Fig. IV.10. The upper bound for the bias in this case is $\delta p_o = 2.2\cdot10^{-4}$ which is 1.1 % of the true value i.e. about 3 times as high as in case 7. This illustrates well that the bias increases if the statistical accuracy of the measurement gets poorer. The fact that the estimate for a_2 happens to be nearer to the true value than in case 7 must not mislead us. This is a mere chance.

The example shown in Figs. IV.11 and IV.12 is case 9 which has a weaker transient term than the previous examples. Both the φ- and Fisher tests recommend step 9 as asymptotic i.e. $x_i \leq 79$. The parameter estimate is $\tilde{a}_2=(1.998\pm0.011)\cdot10^{-2}$. It is remarkable that this asymptotic region is the same as for case 7 although the effect of the transient term is surely greater in the latter case.

As the last example, the results for case 10 were plotted in Fig. IV.13. The fitting function was

$$f(x,\underline{a}) = a_1 e^{-a_2 x} + a_3. \qquad /IV.6.2/$$

The results presented in Figs. IV.13c and d correspond to a_2 as p_ℓ. The

asymptotic region recommended by the test is $x_i \geq 5$ corresponding to step 3. The y_i values were plotted in Fig. III.6. The final parameter estimate is $\tilde{a}_2$=0.1053 $\pm$ 0.001. The confidence interval for ε=0.01 is (0.1027,0·1080). The true value of a_2 is 0.1. This means that our test recommended too large an estimate. The upper bound for the bias is $\delta p_o = 1.1 \cdot 10^{-3}$. The systematic error in our estimate $\tilde{a}_2$ = 0.1053 is even larger than this. We cited this example just to show that the δp_o derived in section IV.4 is only an average of the systematic errors appearing or missing in individual cases. In case 10, it is a "bad luck" that a relatively large systematic error remained in $\tilde{a}_2$ which would be compensated for if the same measurement and fitting were repeated several times. Then there will be cases in which this systematic error will be missing thus leading to a significantly lower bias on the long run.

Finally, Table IV.2 compares the values of Student fraction t_ℓ for ℓ = 1 and t_i for the "most transient" point in step 1. These values are always very near to each other for a given case. Without any theoretical justification, this clearly shows that the stepwise fractions (t_ℓ) and the pointwise fraction (t_i) bear practically the same information concerning the significance of the transient tendencies.

Table IV.2

case	stepwise	pointwise
7	40.95	43.49
8	11.50	14.19
9	13.45	13.97
10	13.98	13.52

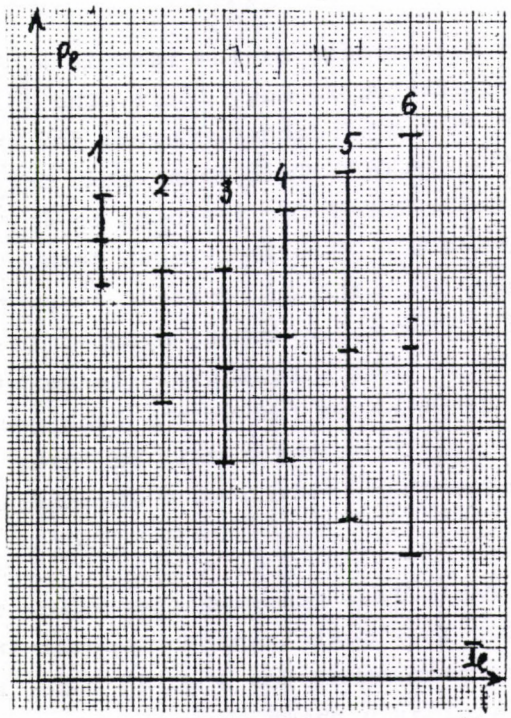

Fig. IV.1

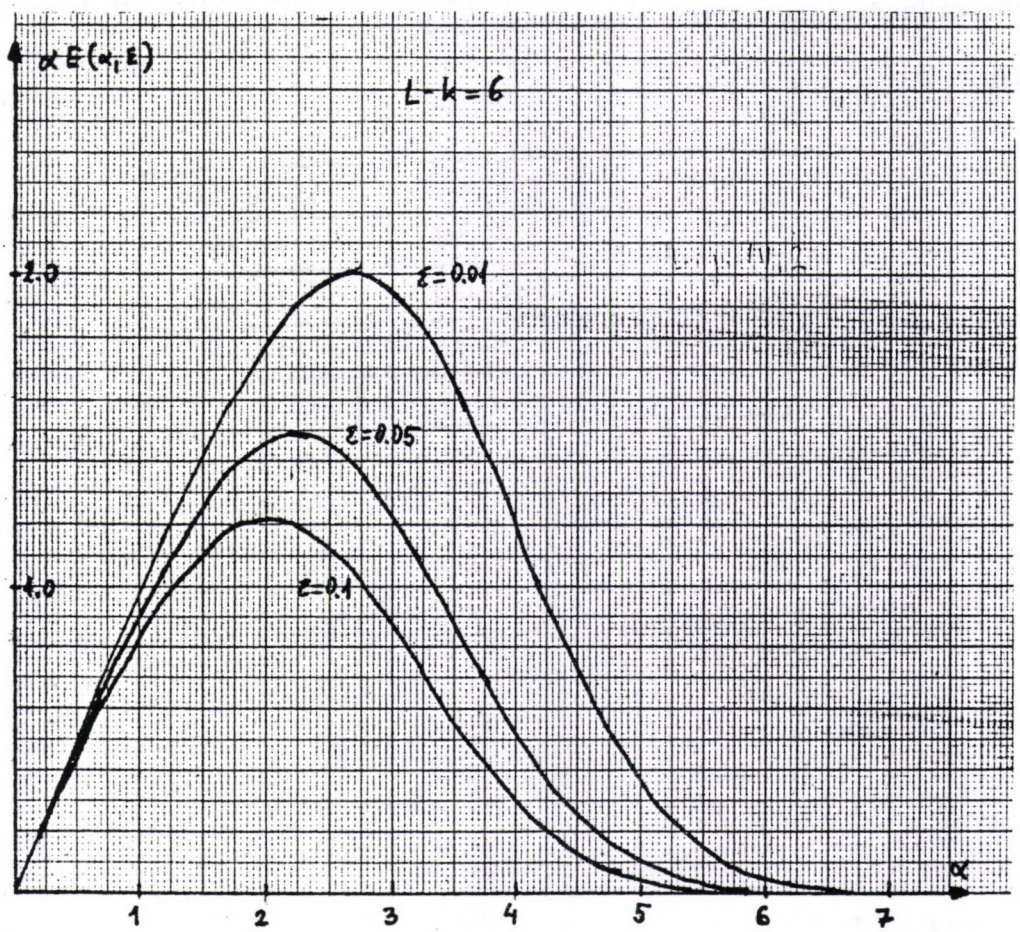

Fig. IV.2

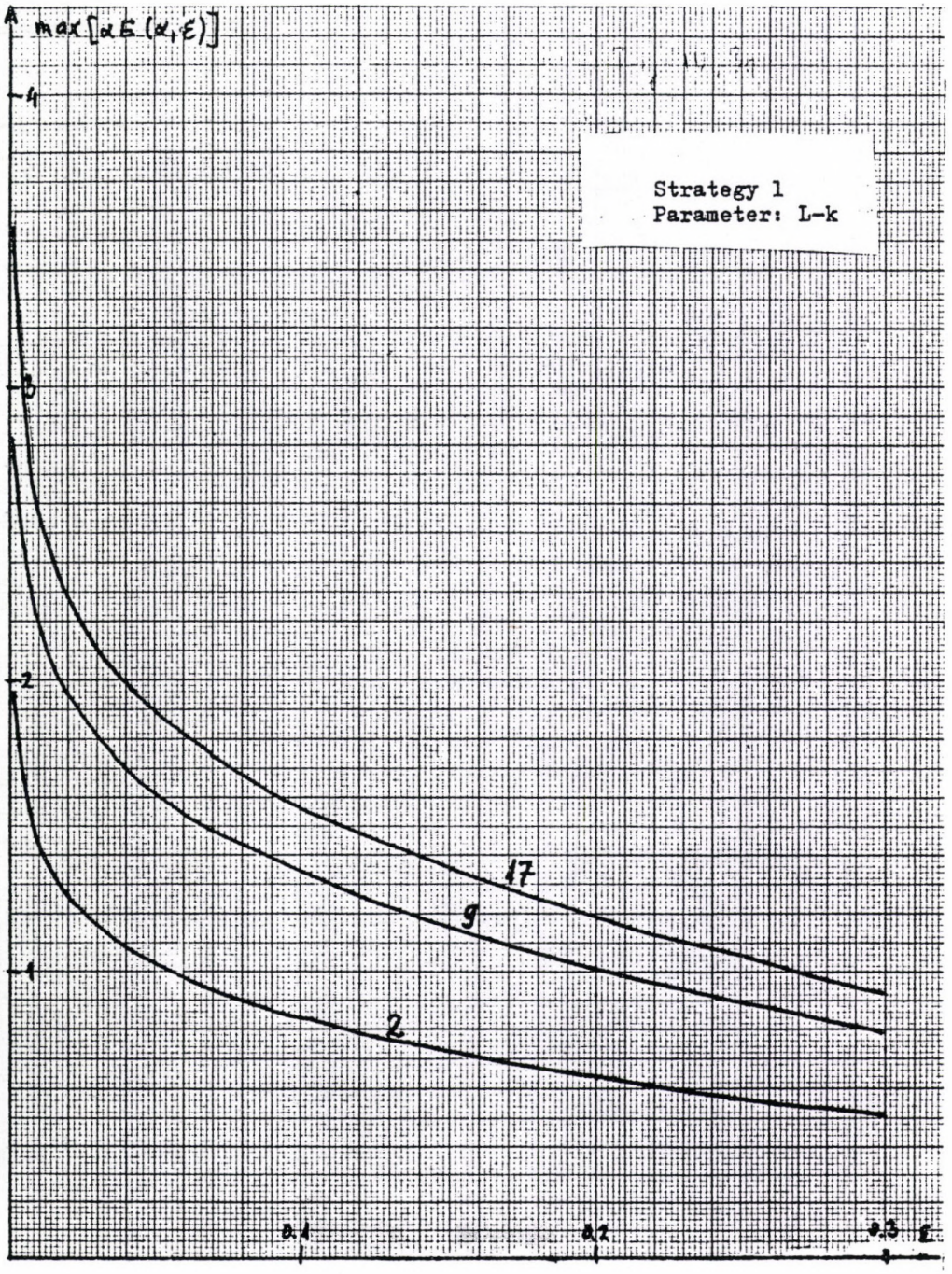

Fig. IV.3a

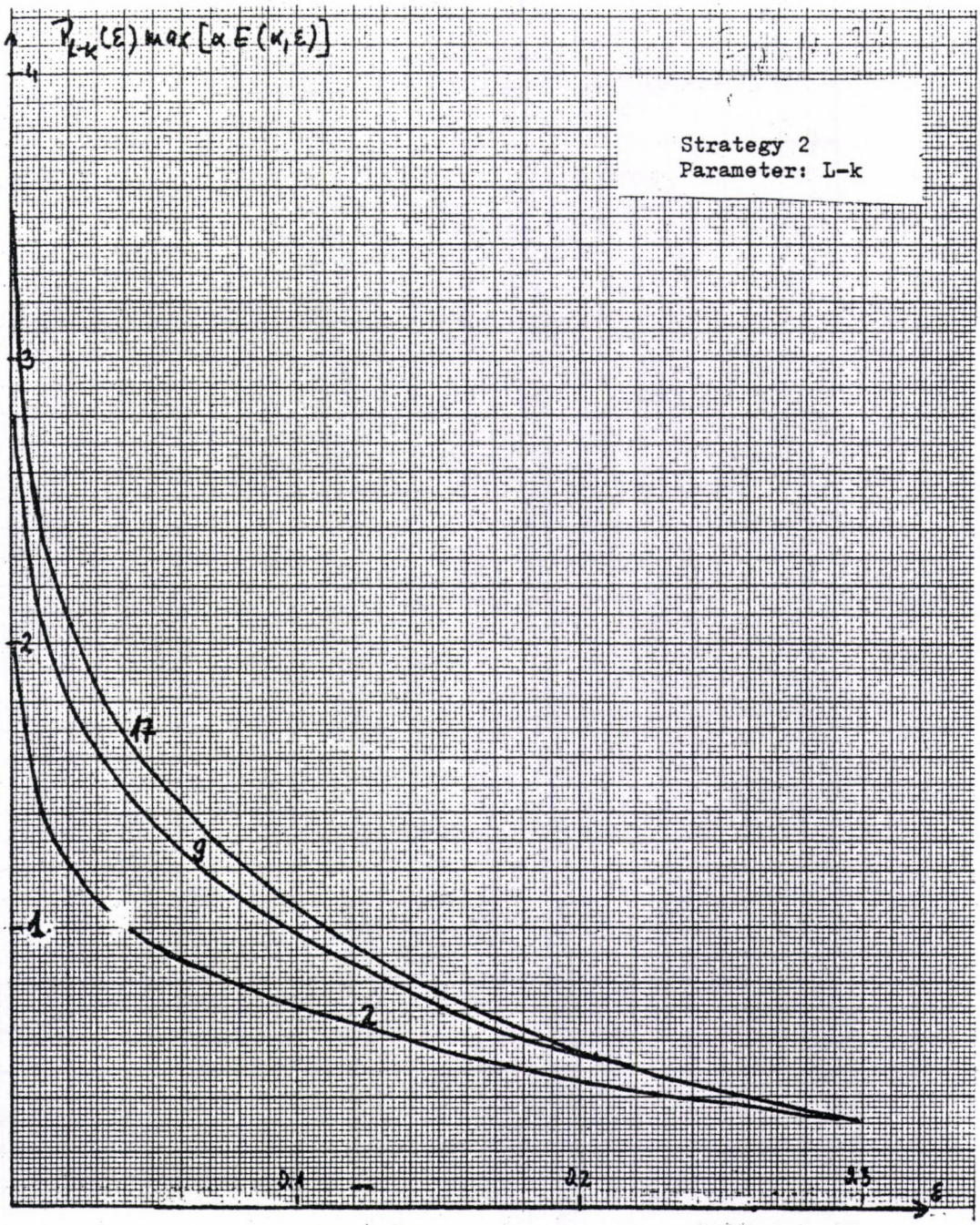
$P_{L-k}(\varepsilon)\ max\ [\alpha\, E(\alpha,\varepsilon)]$
Strategy 2
Parameter: L-k
4
3
2
1
17
9
2
0.1
2.2
3.5
ε

Fig. IV.3b

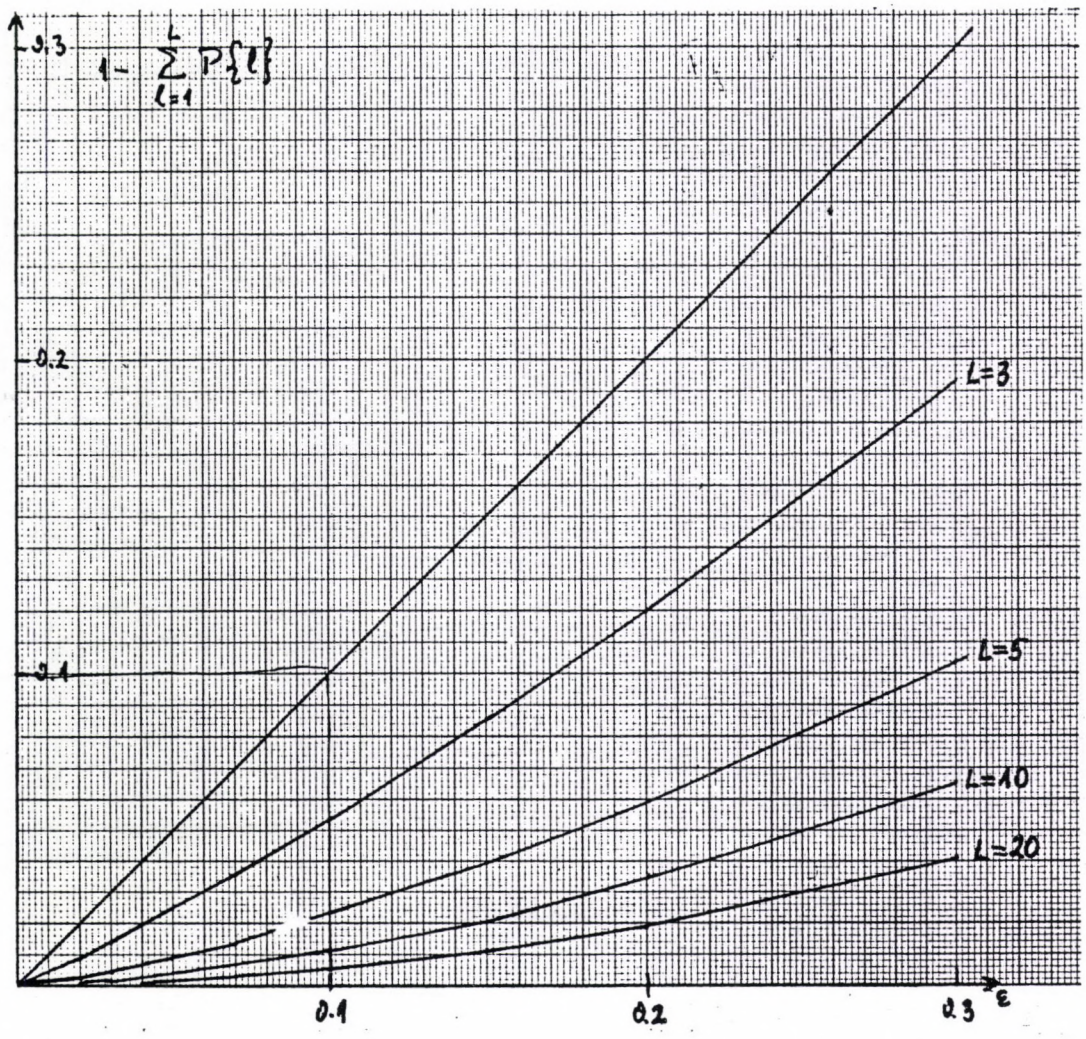

Fig. IV.4

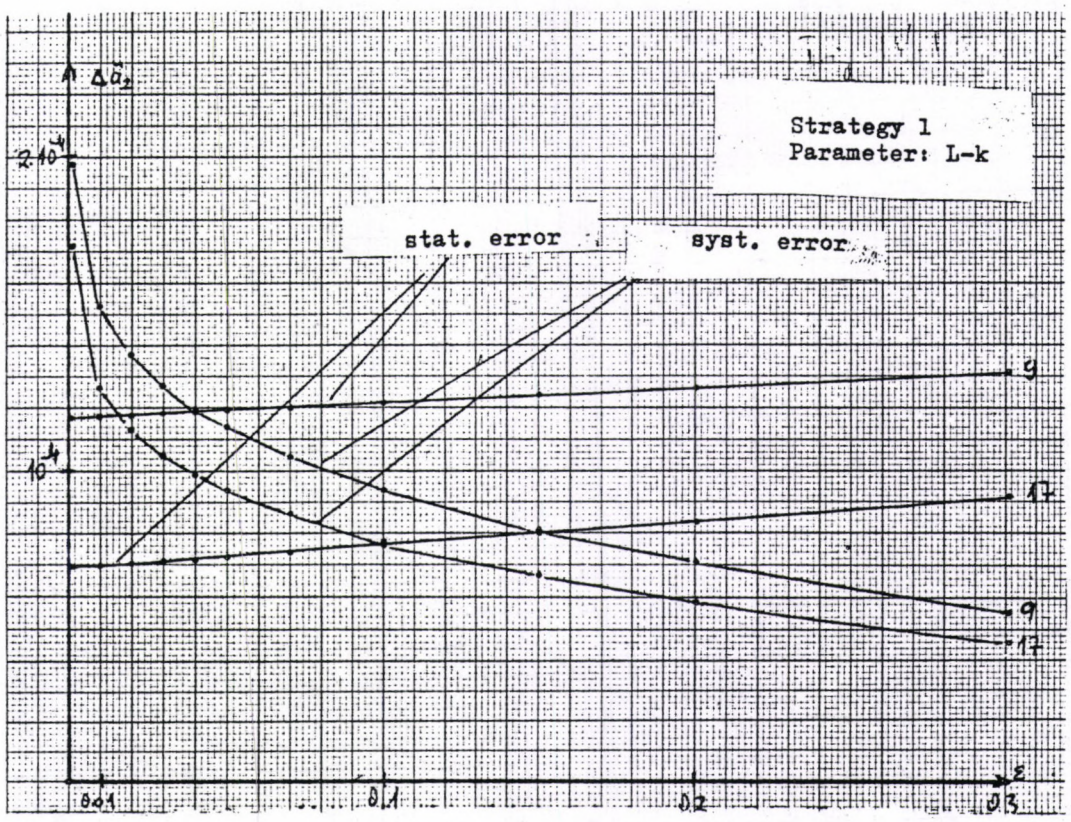
Strategy 1
Parameter: L-k
stat. error
syst. error
9
17
9
17
ε
0.1
0.2
0.3

Fig. IV.5a

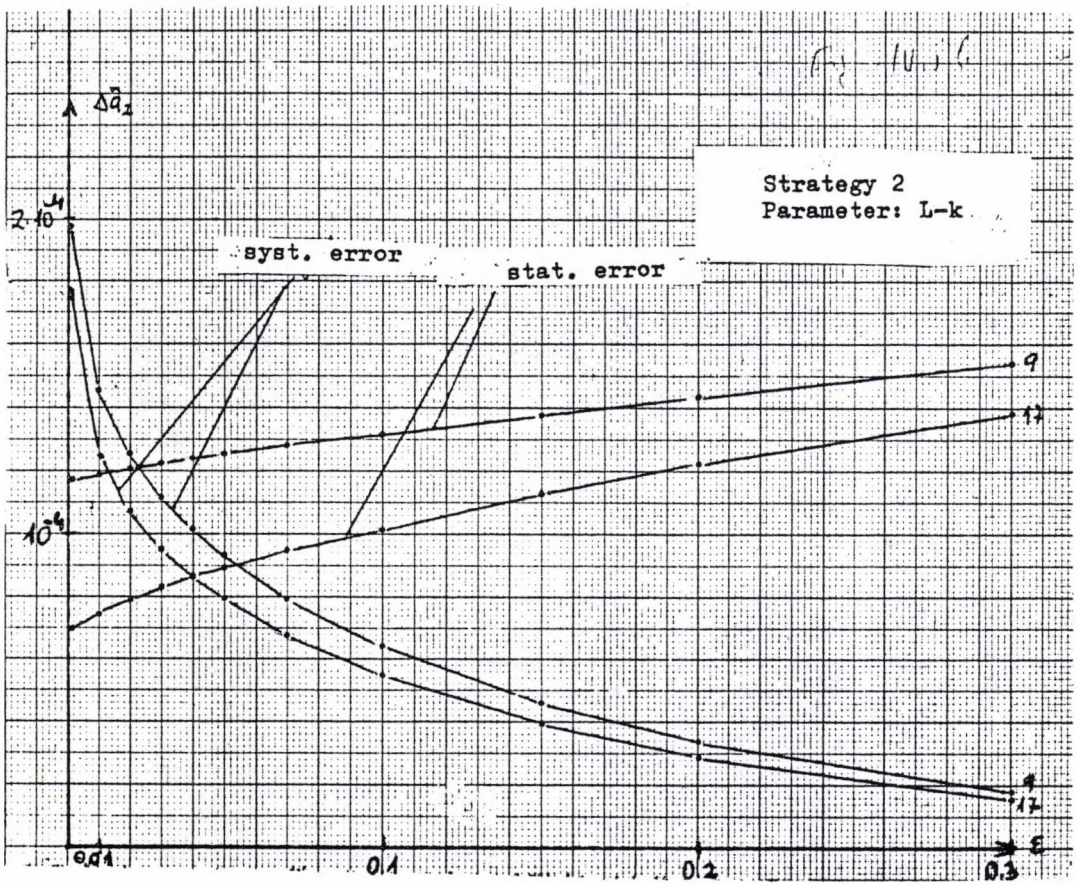

Fig. IV.5b

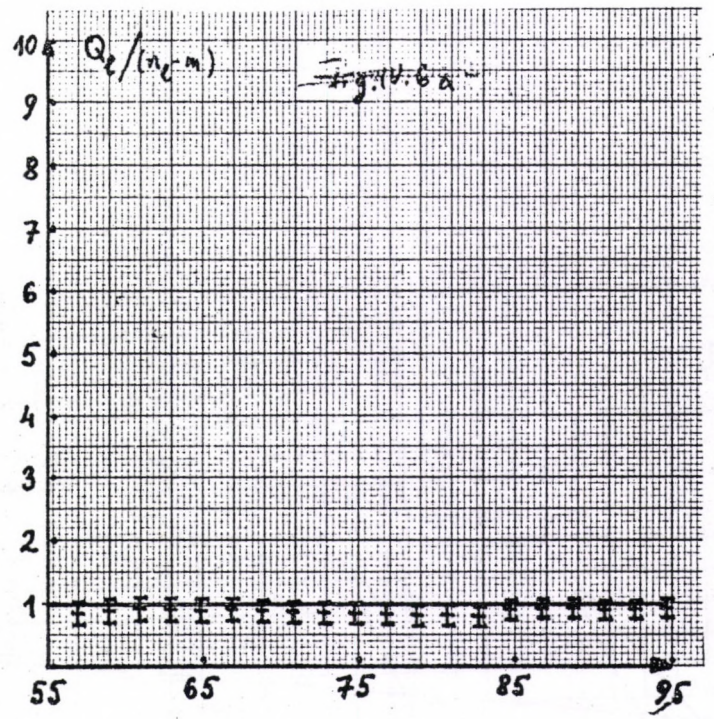

Fig. IV.6a

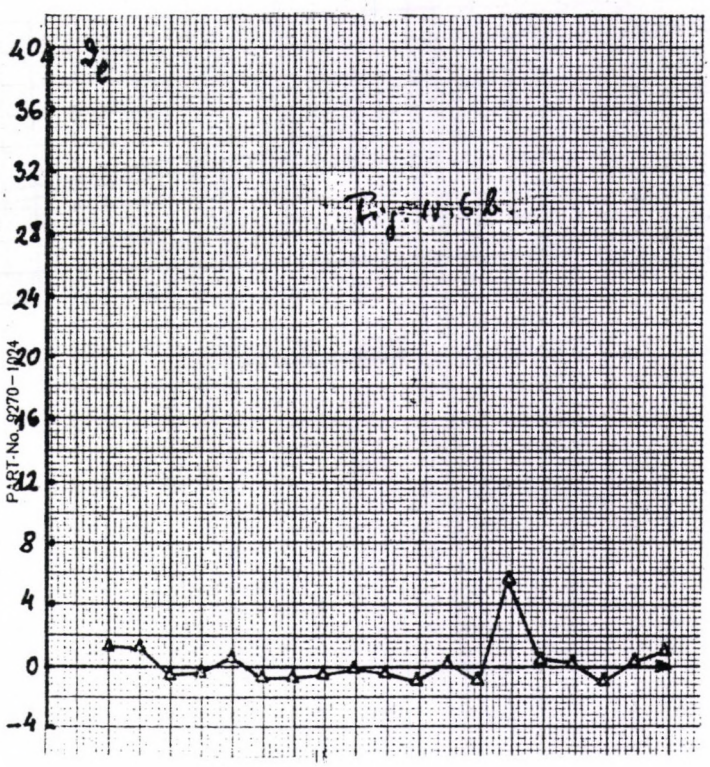

Fig. IV.6b

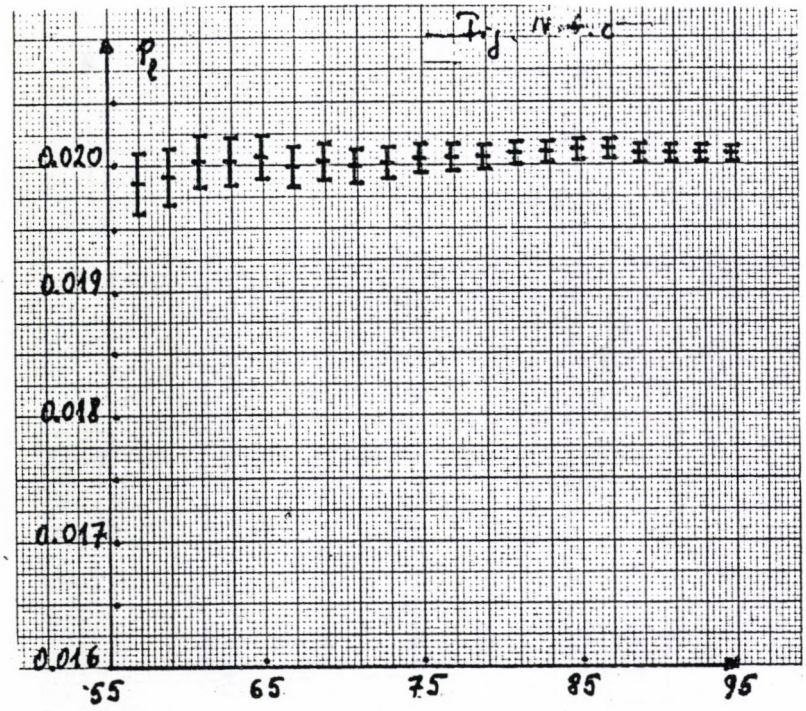

Fig. IV.6c

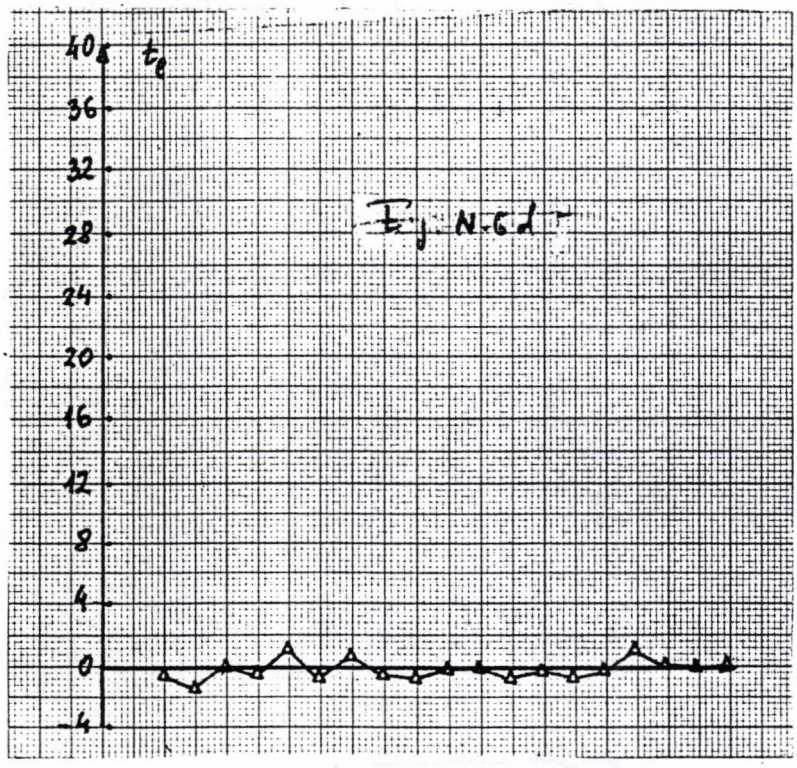

Fig. IV.6.d

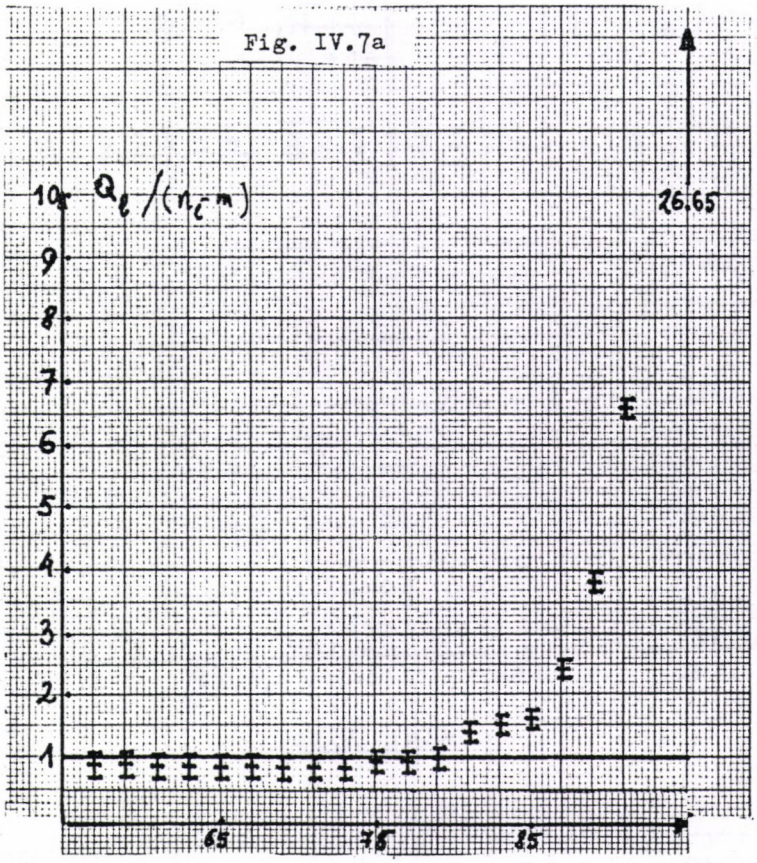

Fig. IV.7a

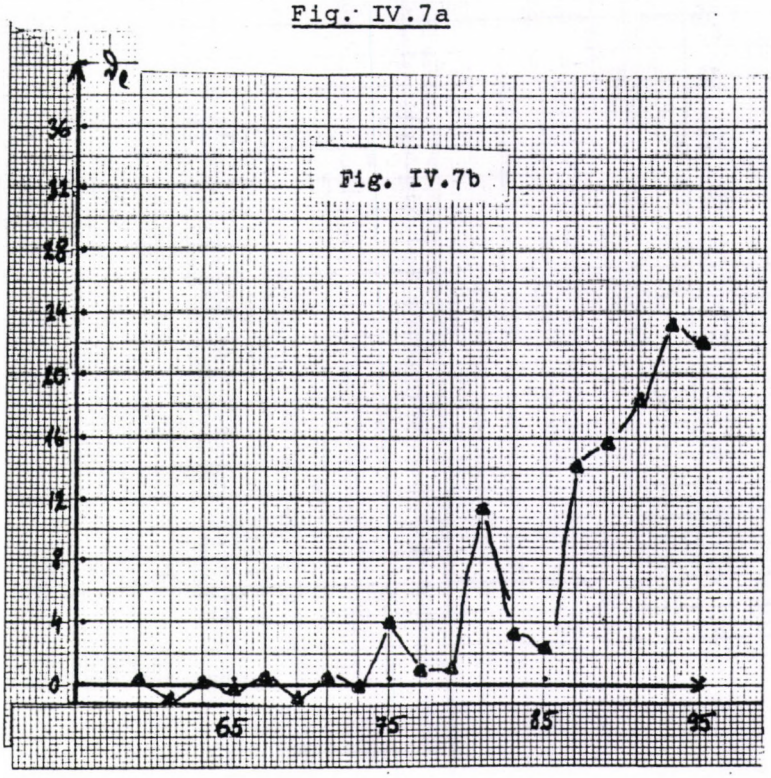

Fig. IV.7b

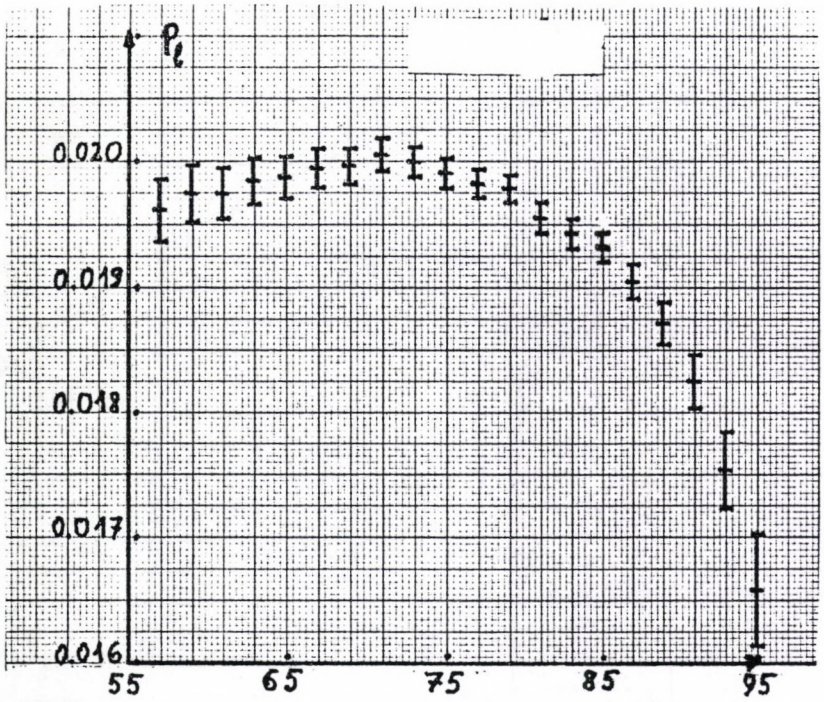

Fig.- IV.7c

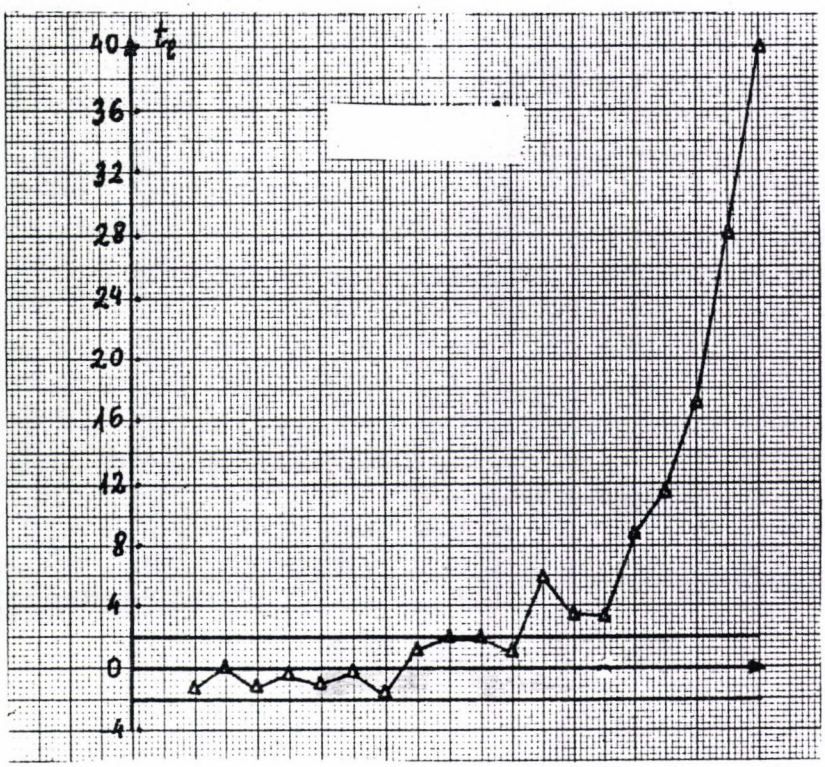

Fig. IV.7d

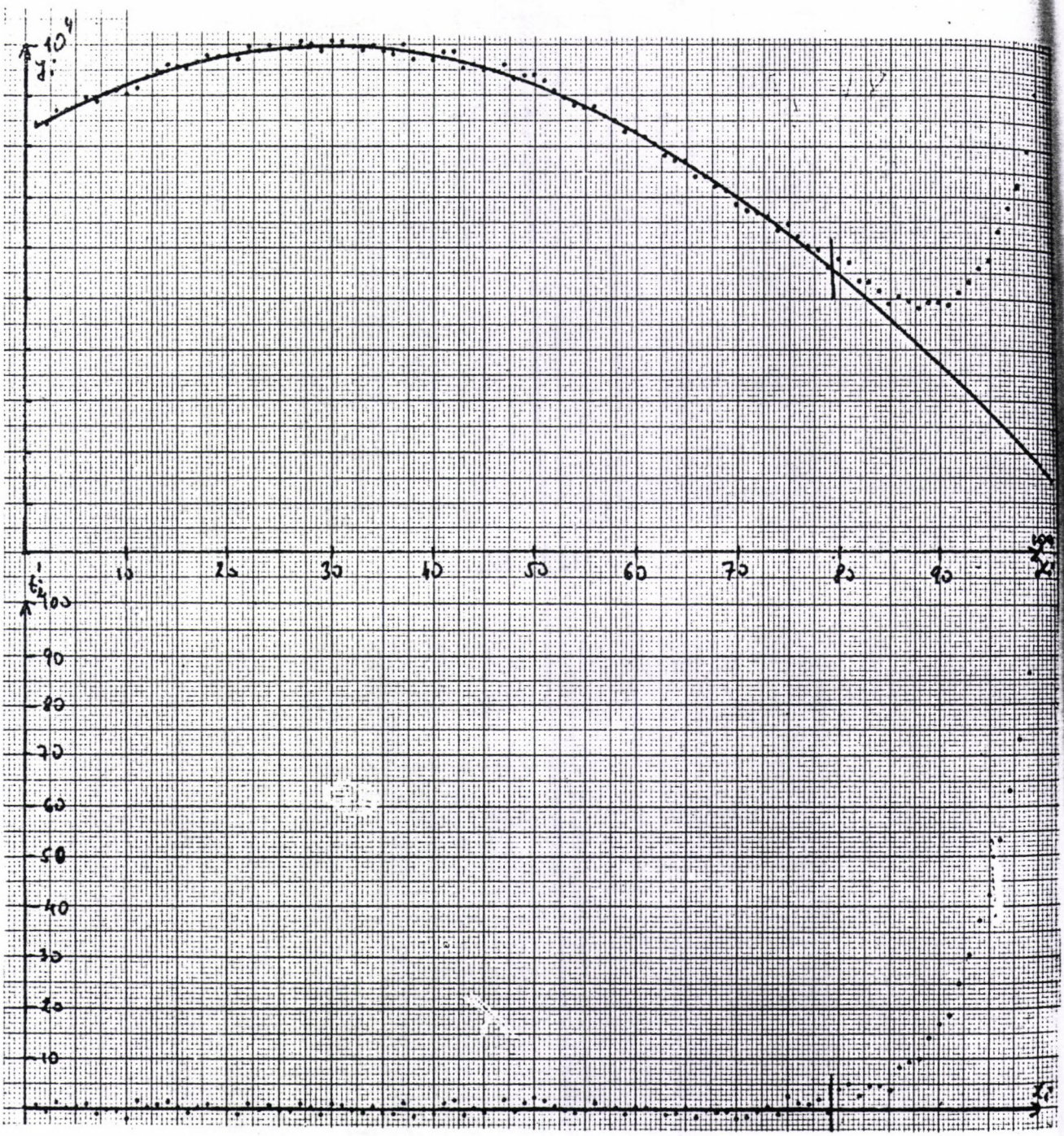

Fig. IV.8

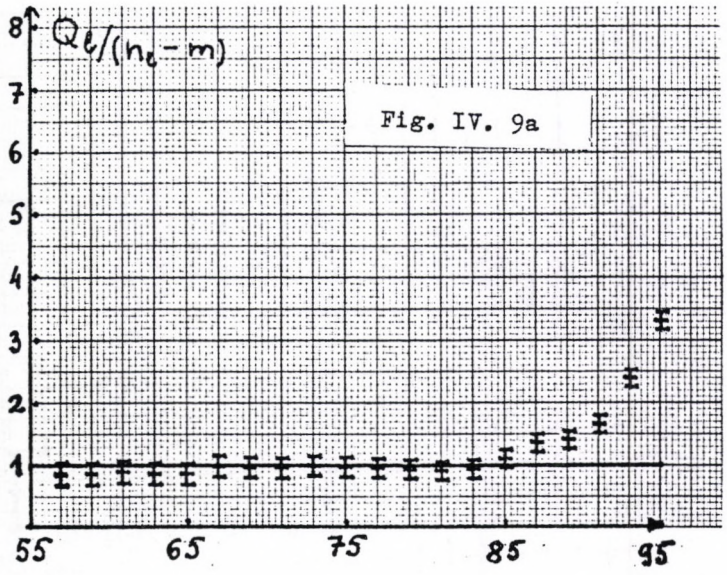

Fig. IV.9a

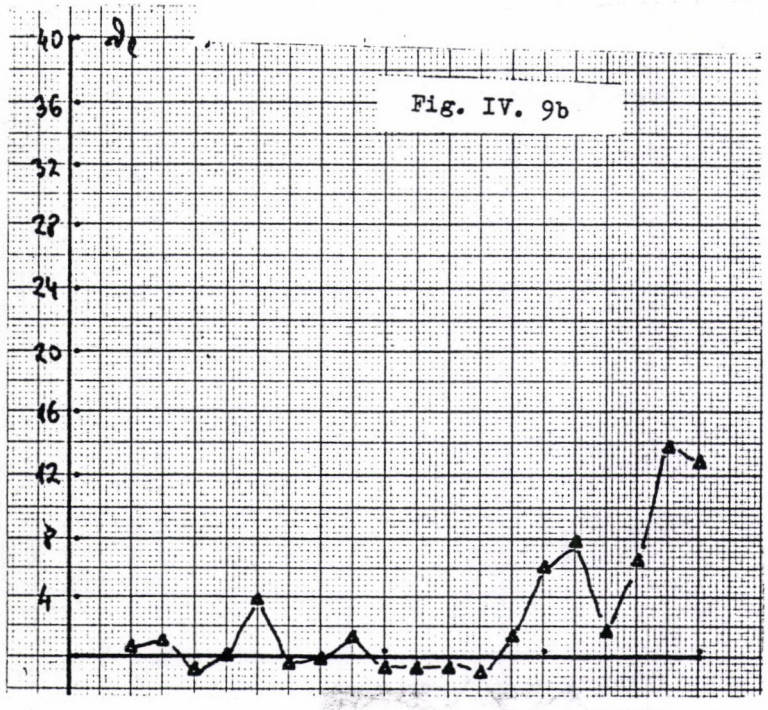

Fig. IV.9b

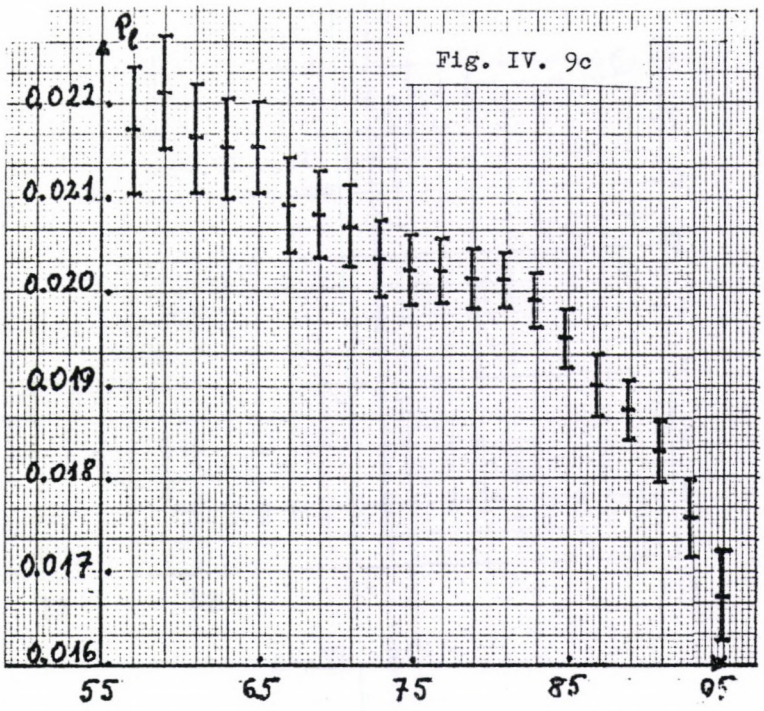

Fig. IV.9c

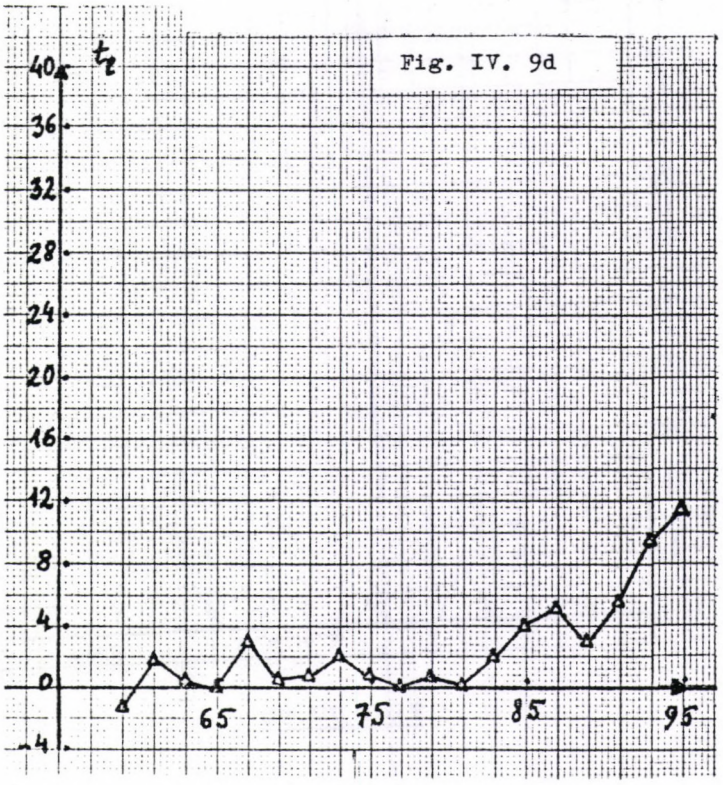

Fig. IV.9d

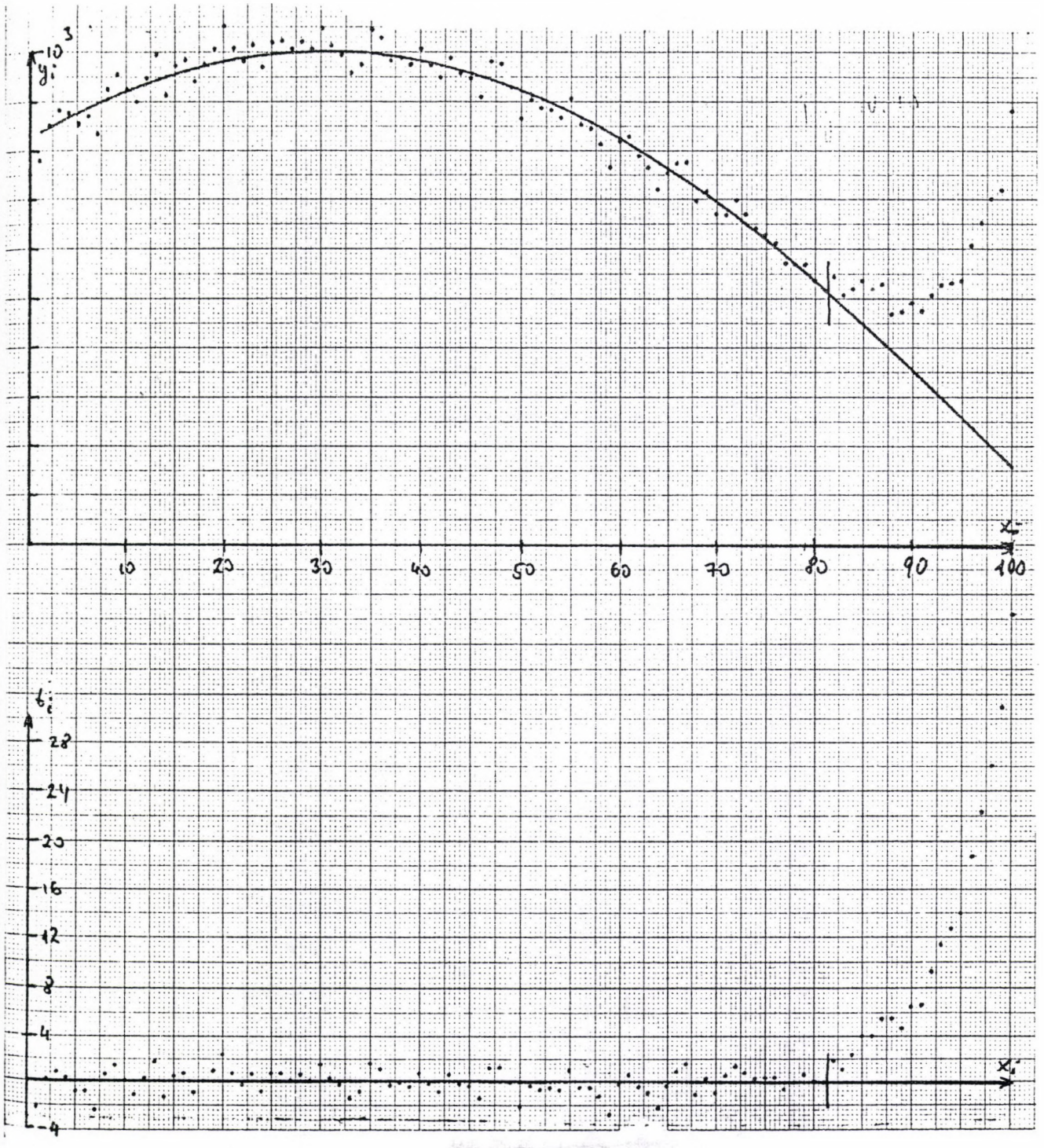

Fig. IV.10

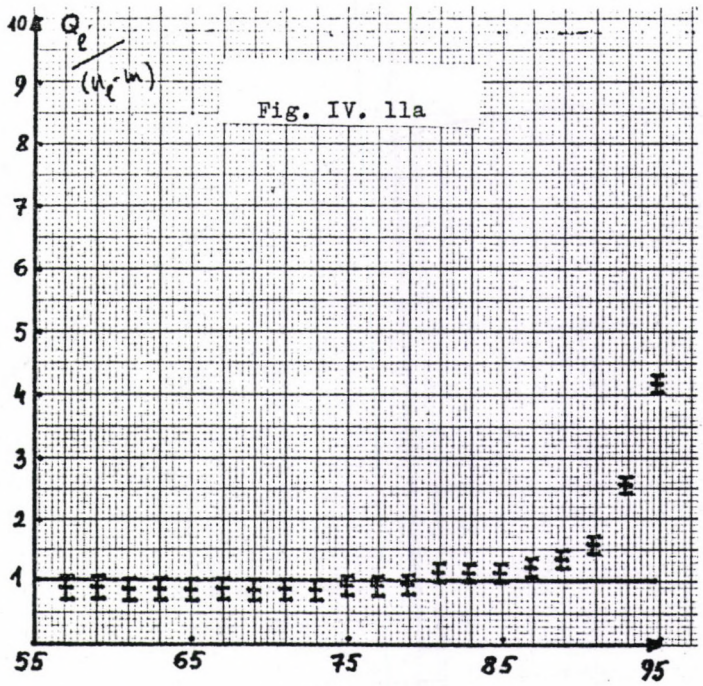

Fig. IV.11a

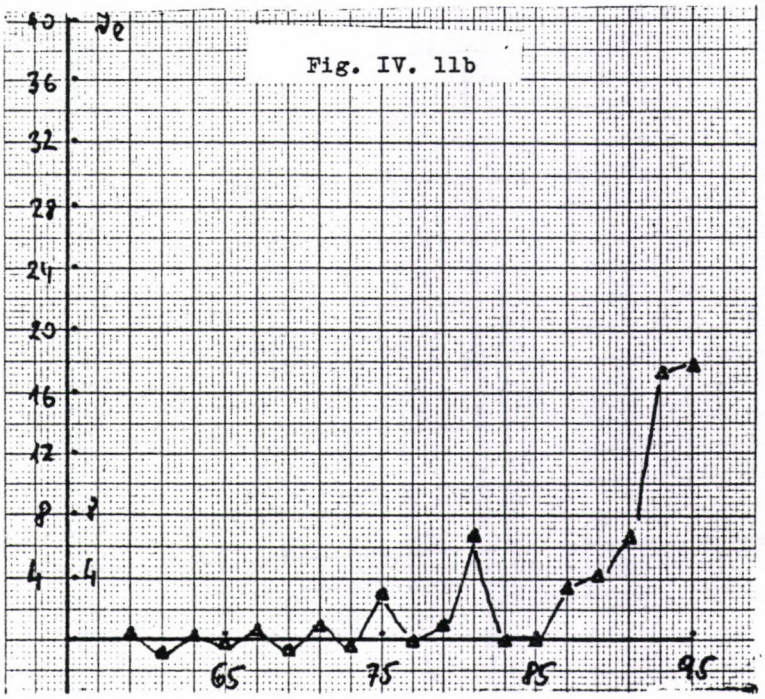

Fig. IV.11b

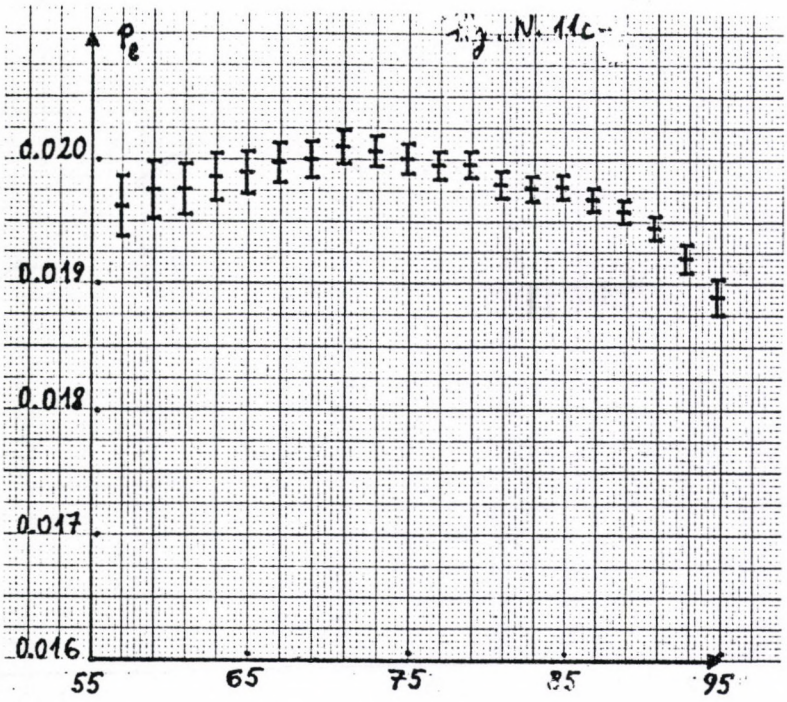

Fig. IV.11c

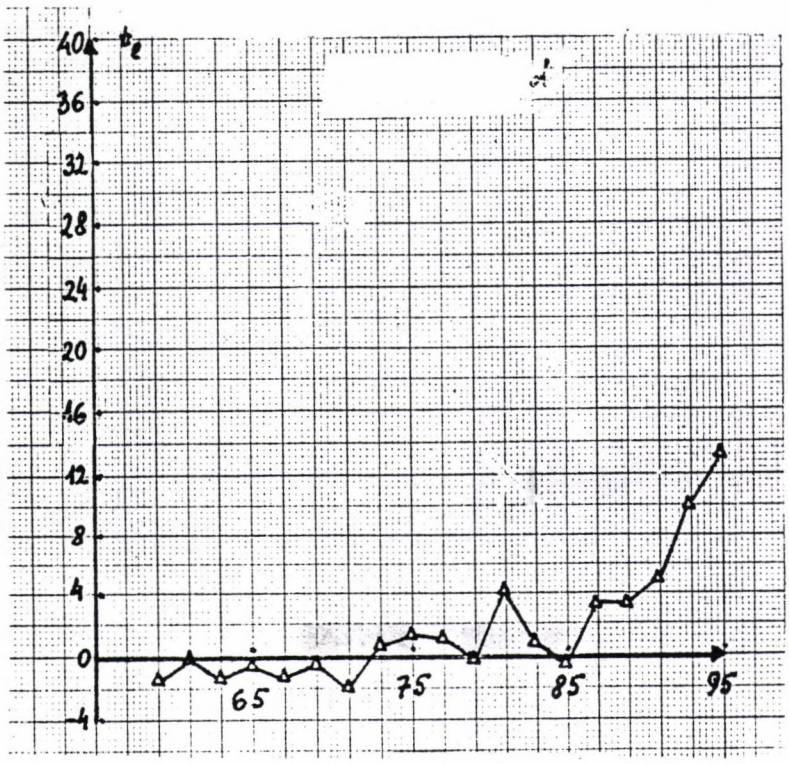

Fig. IV.11d

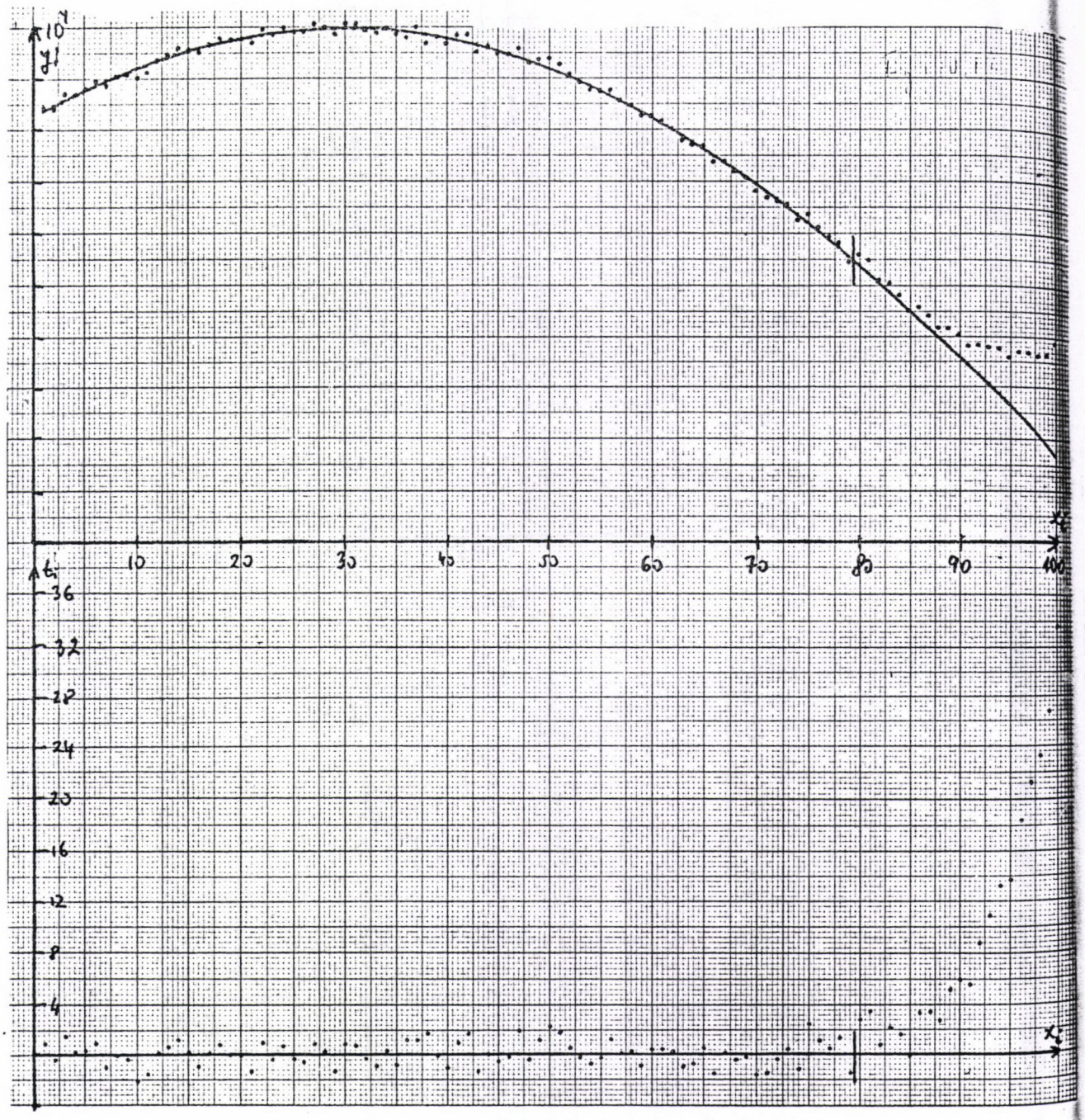

Fig. IV.12

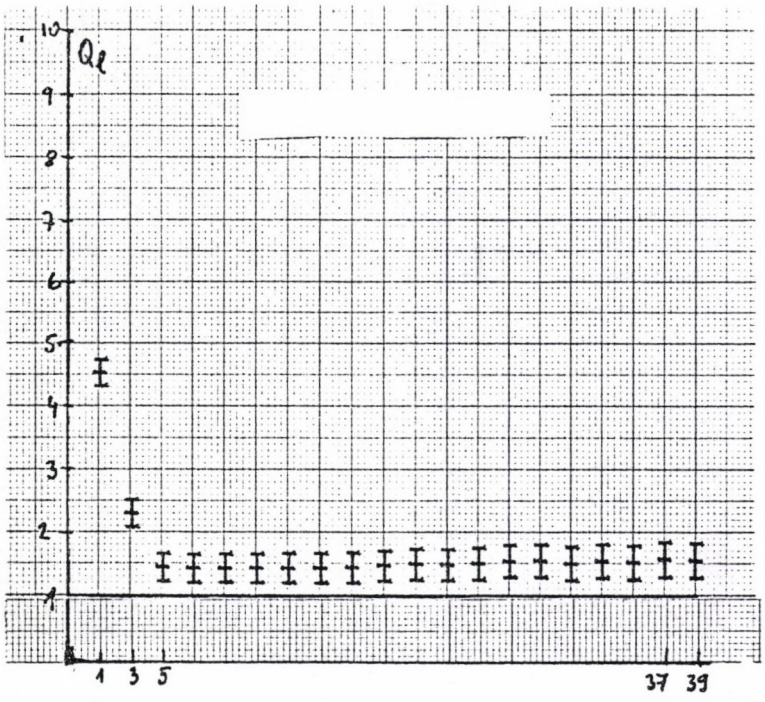

Fig. IV.13a

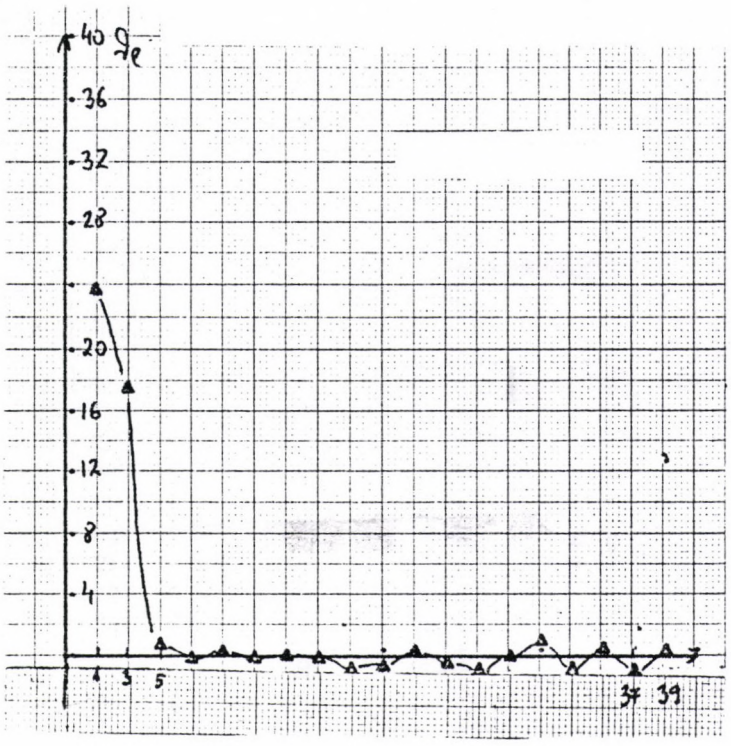

Fig. IV.13b

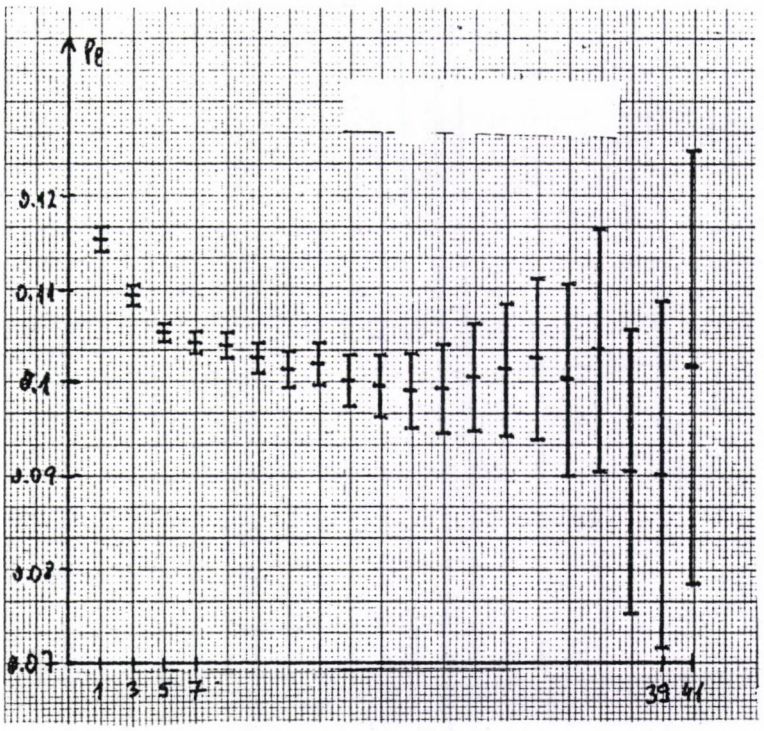

Fig. IV.13c

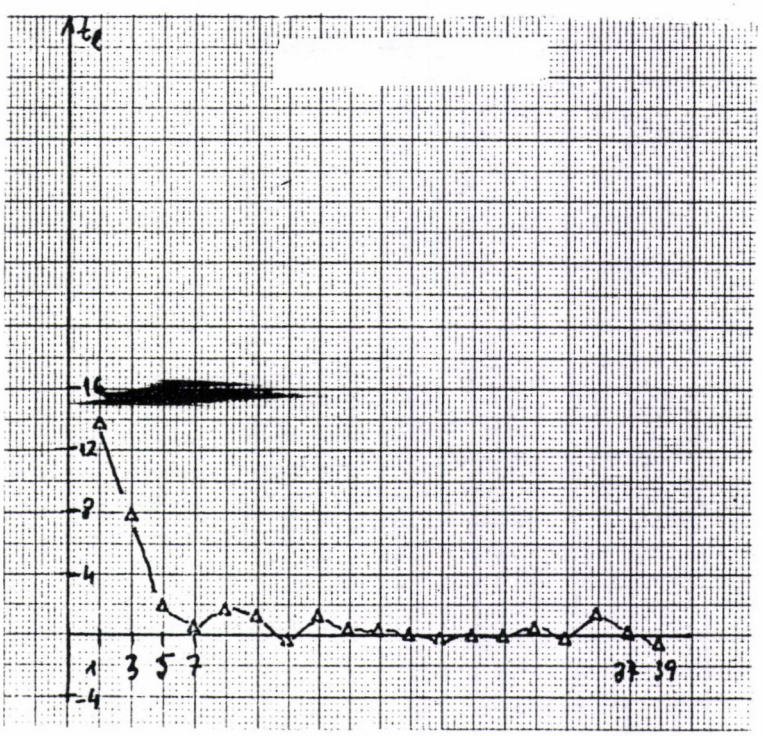

Fig. IV.13d

CHAPTER V

MISCELLANEOUS TOPICS

The choice of the fitting function $f(x,\underline{a})$ represents our knowledge on the physics of the measurements. Our considerations were up to now general from this point of view. In the present chapter, some questions are treated which are connected with the form of $f(x,\underline{a})$. The first of them concerns the corrections /section V.1/ while the second one is the treatment of independently repeated measurements /sections V.2 and V.3/.

V.1 Corrections

In most cases, rough experimental data need be corrected for dead time, radioactive decay, background etc. According to the general practice, these corrections are applied to the primarily measured data and the resulting values are then given to fitting as y_i. This is acceptable in some cases but only under the condition that the errors of the different corrections are propagated along with the corrections and the resulting errors are given as Δy_i. The error propagation requires so many computations that it could rarely be done correctly by hand. These preparatory computations are therefore frequently carried out on small size computers by special programs and their outputs are used as input of the final fitting program.

Program RFIT accepts such data but there is an alternative way of doing the evaluation. All the corrections may be included in $f(x,\underline{a})$ and the fitting is done with the primarily measured data. The basic formulation of RFIT corresponds to this approach. Before discussing the advantages of this, let us look at its details. We shall distinguish two kinds of corrections:

- multiplicative corrections such as measuring time, decay, foil calibration, detector efficiency etc. and
- additive corrections such as background, residual activity etc.

We denote the product of all multiplicative correction factors by μ_i and the sum of all additive corrections by α_i to be applied to the primarily measured value y_i. The dead time correction ν_i considered in section I.2.4 is not included in μ_i.

The corrected value now is

$$y_i^c = \frac{\nu_i y_i - \alpha_i}{\mu_i} \qquad /V.1.1/$$

its variance being

$$\langle(\Delta y_i^c)^2\rangle = \frac{\nu_i^2\sigma_{yi}^2 + \sigma_{\alpha i}^2 + y_i^{c2}\sigma_{\mu i}^2}{\mu_i^2} \qquad /V.1.2/$$

where $\sigma_{\alpha i}^2$ and $\sigma_{\mu i}^2$ are the variances of α_i and μ_i, respectively. The corrected values y_i^c are already very important intermediate results. For example, in case of the macroflux measurement, they give, as a function of the coordinates, the macroflux distribution itself to which a cosine or a Bessel-function may then be fitted. The y_i^c data are generally further reduced by averaging the y_i^c belonging to the same geometrical point. The fitting may, of course, be carried out also with these data. /The question of corrected and averaged distributions will be taken up in section V.2.3./.

In the following, we denote by $g(z_i,\underline{a})$ that fitting function which is used when fitting to y_i^c. In our approach, we do the fitting with the directly measured data /i.e. with y_i/ and include the corrections in the fitting function as

$$f(x_i,\underline{a}) = \frac{\mu_i\, g(z_i,\underline{a}) + \alpha_i}{\nu_i} \qquad /V.1.3/$$

where x_i is now a global notation for variables z_i, μ_i, α_i. Even if z_i may be assumed as a constant, the correction factors μ_i and α_i are surely random variables. In section I.2.2, it was shown how this can be taken into account by chosing weights w_i according to eqs. /I.2.22a/ or /I.2.8b/. Using these formulae, we get that the proper weighting is

$$\frac{\sigma^2}{w_i} = \sigma_{y_i}^2 + \sigma_{z_i}^2\left[\frac{\mu_i}{\nu_i}\,\frac{\partial g(z_i,\underline{a})}{\partial z_i}\right]^2 + \frac{\sigma_{\alpha_i}^2 + \sigma_{\mu_i}^2\left[g(z_i,\underline{a})\right]^2}{\nu_i^2} \approx$$

$$\approx \frac{\mu_i^2}{\nu_i^2}\left(\langle(\delta y_i^c)^2\rangle + \sigma_{z_i}^2\left[\frac{\partial g(z_i,\underline{a})}{\partial z_i}\right]^2\right) \qquad /V.1.4/$$

if $g(z_i,\underline{a})$ is set equal to y_i^c. Inserting this weighting in eq. /I.2.4/, we obtain, after some algebra, the following minimum condition:

$$Q(\underline{a}) = \sum_{i=1}^{n} \frac{\left[y_i^c - g(z_i,\underline{a})\right]^2}{\langle(\Delta y_i^c)^2\rangle + \sigma_{z_i}^2\left[\frac{\partial g(z_i,\underline{a})}{\partial z_i}\right]^2} = \min \qquad /V.1.5/$$

which is the same as fitting function $g(z_i,\underline{a})$ to the corrected values y_i^c.

We have shown herewith that it is theoretically all the same whether we perform the corrections according to eqs. /V.1.1/ and /V.1.2/ before the fitting or we include them in the fitting procedure according to eqs. /V.1.3/ and /V.1.4/ if otherwise the necessary conditions formulated in chapters I and II are met. We return to the question of these conditions later but we discuss some practical points before. In case of fulfilment of these conditions, it seems to be a question of taste which one of these two approaches is chosen. It depends rather on the ultimate purpose of the evaluation or, in other words, on what we intend to do with the final results and conclusions of it.

- The calculation of the corrected y_i^c values is always necessary. As stated above, only they have some physical significance since the corrections take care only of the laboratory conditions of the measurements.
- Including the corrections in the fitting function according to eq. /V.1.3/ and working with primarily measured data are convenient from both practical and theoretical points of view. This approach is practically advantageous because one preparatory step /namely the calculation of y_i^c/ is omitted. After performing the fitting, it is not late yet to let the fitting program calculate the y_i^c. There is, however, a less obvious practical advantage, too. When the statistical analysis of the data finds some value to be defective, it is easier to identify the cause of this if the evaluation is based on primary data.
- The theoretical convenience consists in that the theoretical derivations are simpler if the fitting function is defined according to eq. /V.1.3/. Furthermore, the possibilities of this approach are broader. As we shall see later, this approach works even in cases when the other one practically fails.

V.1.1 Correlated corrections

The minimum of the sum of squares $Q(\underline{a})$ defined by eq. /V.1.5/ may be found by the techniques described in section I.3 so that this minimum condition will yield an estimate for $\underline{a}$. In the analysis of the statistical properties of such estimates, it was an essential condition that the y_i^c are statistically independent i.e. that eq. /II.1.3/ holds. The primary experimental data y_i may be assumed as independent but the correction factors are not necessarily so.

The simplest example is the case of a constant, independently measured background. In our notations, this corresponds to the case when the α_i are the same for all i. It is clear that this leads to the following covariances:

$$\langle (\Delta y_i^c \; \Delta y_i^c,) \rangle = \frac{\sigma_\alpha^2}{\mu_i \mu_i,}, \qquad /V.1.6/$$

Under normal conditions, the background is small so that both σ_α^2 and these covariances play a not too important role. This is true but the point is that it is always advisable to be aware of what we are neglecting.

In the next example, the covariances are always important although they are generally neglected. The radioactive decay of a single isotope is exponential and the decay correction is done according to an exponential formula. If the decay constant may not be assumed to be known accurately i.e. it is a random variable, this leads to a covariance analogous to that given in eq. /V.1.6/. Writing

$$\mu_i = e^{-\lambda t_i}$$

where λ is the decay constant and t_i is the time when y_i was measured, differentiation of eq. /V.1.1/ yields that

$$\langle \Delta y_i^c \Delta y_i^c, \rangle = \frac{\nu_i y_i}{\mu_i} \frac{\nu_i, y_i,}{\mu_i,} t_i t_i, \sigma_\lambda^2 \qquad /V.1.7/$$

where σ_λ^2 is the variance of λ.

When measuring the activity of Pu or U foils or when performing a γ-scanning of irradiated fuels, the measured activities do not decay exponentially. In such cases, a monitor element /a foil or a special fuel element/ is used for determining the time dependence of the decay. Its activity is measured from time to time. According to the general practice, each third measurement is a monitor activity. The decay correction factors μ_i may then be obtained for example by logarithmic interpolation of the monitor activities. Let us suppose that we have the monitor activites m_1 and m_2 measured in times t_1 and t_2, respectively, and we need the decay correction $\mu(t)$ for the time t $(t_1<t<t_2)$. The logarithmic interpolation yields

$$\log \mu(t) = \frac{t_2-t}{t_2-t_1} \log m_1 + \frac{t-t_1}{t_2-t_1} \log m_2 \qquad /V.1.8/$$

leading to a covariance of different correction factors /say $\mu(t)$ and $\mu(t')$/

$$\langle (\Delta\mu(t) \; \Delta\mu(t')) \rangle = \frac{\mu(t)\mu(t')}{(t_2-t_1)^2} \left[\frac{\sigma_{m_1}^2}{m_1^2}(t_2-t)(t_2-t') + \frac{\sigma_{m_2}^2}{m_2^2}(t-t_1)(t'-t_1) \right] \qquad /V.1.9a/$$

if $\mu(t')$ is also interpolated from m_1 and m_2 according to eq. /V.1.8/. If, however, $\mu(t')$ is obtained from m_2 and m_3 measured in times t_2 and t_3,

respectively, $(t_2<t'<t_3)$, i.e.

$$\log \mu(t') = \frac{t_2-t'}{t_2-t_3} \log m_3 + \frac{t'-t_3}{t_2-t_3} \log m_2,$$

the covariance is given by the formula

$$<(\Delta\mu(t)\Delta\mu(t'))> = \frac{\mu(t)\mu(t')}{(t_2-t_1)(t_2-t_3)} \frac{\sigma m_2^2}{m_2^2} (t-t_1)(t'-t_3). \qquad /V.1.9b/$$

$\mu(t)$ and $\mu(t')$ are independent if their respective (t_1, t_2) interpolation intervals are disjoint. Setting $t=t'$ in eq. /V.1.9a/, we get the variance of $\mu(t)$ as

$$\sigma^2_{\mu(t)} = \frac{\mu(t)^2}{(t_2-t_1)^2} \left[\frac{\sigma_{m_1}^2}{m_1^2} (t_2-t)^2 + \frac{\sigma_{m_2}^2}{m_2^2} (t_1-t)^2 \right] . \qquad /V.1.10/$$

In practical cases, the covariances just calculated are always very close to the variances.

These simple formulae are useful when writing programs including corrections but now we look at them at a different angle. The examples presented above show that the covariance matrix of the correction factors can be simply calculated so that it may be assumed as known. In the following, we intend to study the consequences of the presence of off-diagonal elements of this matrix. For simplicity, we suppose for the moment that the additive corrections are independent and are already included in y_i according to eqs. /V.1.1/ and /V.1.2/. Similarly, the dead time correction is meant to be included in $g(z_i,\underline{a})$. Let us denote the covariance matrix of the μ_i values by $\underline{\underline{C}}$, i.e.

$$C_{ii'} = < \Delta\mu_i \, \Delta\mu_{i'} > \qquad /V.1.11a/$$

and the expectation of μ_i by μ_{io} , i.e.

$$<\mu_i> = \mu_{io} \; . \qquad /V.1.11b/$$

Now the likelihood function of the random variables y_i and μ_i /i=1,2,...,n/ may be written as

$$L(\underline{y},\underline{\mu},\underline{a}) = \text{const. exp} \; \{- \frac{\sigma^2}{2} Q\} \qquad /V.1.12/$$

where

$$Q = \sum_{i=1}^{n} w_i [y_i - \mu_{io} g(z_i,\underline{a})]^2 + \sum_{i=1}^{n} \sum_{i'=1}^{n} \omega_{ii'} (\mu_i-\mu_{io})(\mu_{i'}-\mu_{i'o}) \; . \qquad /V.1.13/$$

Here, ω_{ii}, is an element of matrix $\underline{\underline{C}}^{-1}$ and $\underline{\mu}$ is a vector with μ_i as components. According to the maximum likelihood principle, we have to find the minimum of Q as a function of the unknown parameters which are now a_k /k=1,2,...,m/ and μ_{io} /i=1,2,...,n/. Differentiating Q with respect to a_k and μ_{io}, we get the equations

$$-\frac{1}{2}\frac{\partial Q}{\partial a_k} = \sum_{i=1}^{n} w_i \mu_{io}[y_i - \mu_{io} g(z_i,\underline{a})] \frac{\partial g(z_i,\underline{a})}{\partial a_k} = 0 \qquad /V.1.14a/$$

for $k = 1,2,...,m$

$$-\frac{1}{2}\frac{\partial Q}{\partial \mu_{io}} = \sum_{i'=1}^{n} \omega_{ii'}(\mu_{i'} - \mu_{i'o}) + w_i g(z_i,\underline{a})[y_i - \mu_{io} g(z_i,\underline{a})] = 0 \qquad /V.1.14b/$$

for $i=1,2,...,n$

We are not interested in the determination of the μ_{io}, therefore, we eliminate them from eq. /V.1.14a/. To this end, let us introduce diagonal matrix $\underline{\underline{\Gamma}}$ with $g(z_i,\underline{a})$ as elements and vector $\underline{d}$ with the elements

$$d_i = y_i - \mu_i g(z_i,\underline{a}) = y_i - f(x_i,\underline{a}) \; . \qquad /V.1.15/$$

Furthermore, we remark that $\mu_{io}\partial g(z_i,\underline{a})/\partial z_i$ is the F_{ik} defined by eq. /II.1.1/. With these notations and taking into account the identity

$$y_i - \mu_{io} g(z_i,\underline{a}) = d_i + (\mu_i - \mu_{io}) g(z_i,\underline{a}) \qquad /V.1.16/$$

we simply find from eq. /V.1.14b/ that

$$\underline{\mu} - \underline{\mu}_o = -(\underline{\underline{C}}^{-1} + \underline{\underline{\Gamma}}^2 \underline{\underline{W}}_y)^{-1} \; \underline{\underline{\Gamma}}\underline{\underline{W}}_y \underline{d} \qquad /V.1.17/$$

and eq. /V.1.14a/ may be rewritten as

$$\underline{\underline{F}}^T \underline{\underline{W}}_y \underline{d} + \underline{\underline{F}}^T \underline{\underline{W}}_y \underline{\underline{\Gamma}}(\underline{\mu} - \underline{\mu}_o) = 0.$$

The value of vector $/\underline{\mu} - \underline{\mu}_o/$ may be put in here from eq. /V.1.17/ yielding

$$\underline{\underline{F}}^T \underline{\underline{W}}_y [\underline{\underline{E}} - \underline{\underline{\Gamma}}(\underline{\underline{C}}^{-1} + \underline{\underline{\Gamma}}^2 \underline{\underline{W}}_y)^{-1} \; \underline{\underline{\Gamma}}\underline{\underline{W}}_y] \underline{d} = 0.$$

Taking into account that, being diagonal matrices, $\underline{\underline{\Gamma}}$ and $\underline{\underline{W}}$ commute, this last equation may be transformed as

$$\underline{G}(\underline{a}) = \underline{\underline{F}}^T (\underline{\underline{W}}_y^{-1} + \underline{\underline{\Gamma}}\underline{\underline{C}}\underline{\underline{\Gamma}})^{-1} \; \underline{d} = 0 \; . \qquad /V.1.18/$$

This final formula is a set of m equations only with a_k /k=1,2,...,m/ as unknowns. It may be considered as a generalization of eqs. /I.2.5/ and /I.2.6/. That is why its left hand side was again denoted by $\underline{G}(\underline{a})$. If $\underline{\underline{C}}$ is diagonal i.e. the μ_i are independent from each other, this corresponds to a least squares fitting with the weights defined by eq. /V.1.4/. If, however, the μ_i are correlated, a generalized weighting method has to be used. The weighting matrix has been obtained as $(\underline{\underline{W}}_y^{-1} + \underline{\underline{\Gamma}}\underline{\underline{C}}\underline{\underline{\Gamma}})^{-1}$. As it may be simply seen, this just the covariance matrix of vector $\underline{d}$.

The statistical properties of the solutions of eq. /V.1.18/ may be derived along the lines of section II.1. Just as in section II.1, eq. /V.1.18/ is differentiated and we get that

$$\Delta\underline{a} = \underline{\underline{M}}^{-1}\,\underline{\underline{F}}^T\underline{\underline{U}}(\Delta\underline{y}-\underline{\underline{\Gamma}}\Delta\underline{\mu}) \qquad /V.1.19/$$

where

$$\underline{\underline{U}} = (\underline{\underline{W}}_y^{-1} + \underline{\underline{\Gamma}}\underline{\underline{C}}\underline{\underline{\Gamma}})^{-1} \qquad /V.1.20/$$

and

$$\underline{\underline{M}} = \underline{\underline{F}}^T\underline{\underline{U}}\underline{\underline{F}} \qquad /V.1.21/$$

note that eq. /V.1.19/ is a direct generalization of eq. /II.1.12/. Taking into account that

$$\langle\Delta\underline{\mu}\Delta\underline{\mu}^T\rangle = \sigma^2\,\underline{\underline{C}} \qquad /V.1.22a/$$

and

$$\langle\Delta\underline{y}\Delta\underline{y}^T\rangle = \sigma^2\underline{\underline{W}}_y^{-1} \qquad /V.1.22b/$$

we simply derive the formula for the covariance matrix of vector $\tilde{\underline{a}}$ as

$$\underline{\underline{B}} = \langle\Delta\underline{a}\Delta\underline{a}^T\rangle = \sigma^2\,\underline{\underline{M}}^{-1} \qquad /V.1.23/$$

which is formally identical with eq. /II.1.13/ with the exception that $\underline{\underline{M}}$ is not the same as the $\underline{\underline{M}}$ defined by eq. /II.1.4/.

σ^2 was estimated in eq. /II.3.2/ on the basis of Q_{min}. Eq. /V.1.18/ may be considered as corresponding to the minimum of the quadratic form

$$Q = \underline{d}^T\underline{\underline{U}}\underline{d} = \sum_{i=1}^{n}\sum_{i'=1}^{n} U_{ii'}\,d_i\,d_{i'} \,. \qquad /V.1.24/$$

It may be shown that the minimum of this Q satisfies eq. /II.3.1/. Consequently, our basic results derived in the previous chapters remain valid.

V.1.2 Practical work with correlated corrections

In the previous section, we have found the principal solution of the problem of fitting with correlated corrections but, unfortunately, we have not found the practical solution. The point is that computation with matrices as big as matrix $\underline{\underline{U}}$ would not be convenient. For example, if the number of points is 100, $\underline{\underline{U}}$ is a 100 by 100 matrix for which one generally does not have enough storage capacity for one hand, and the inversion of such big matrices is rather time comsuming, for the other hand.

In order to get out of this situation, let us look at the consequences of omitting the off-diagonal terms from eq. /V.1.24/. This would be just the sum written down already in eq. /V.1.5/. It is also a positive definite quadratic form, hence it is reasonable to search its minimum. The resulting estimates of the unknown parameters a_k , however, will not be maximum likelihood estimates because the latter ones are obtained only when the off-diagonal terms are also taken into account. Consequently, their variances will not be minimal. The maximum likelihood method generally represents a rather broad minimum of the variances so that a slightly different method /namely the solution of eq. /V.1.5// is not expected to lead to much larger parameter variances. In other words, use of eq. /V.1.5/ can be tolerated.

Thus, we returned to a method which is formally identical with the method treated in the previous chapters. Unfortunately, formula /II.1.13/ does not remain valid. Let us write matrix $\underline{\underline{U}}^{-1}$ as the sum of two matrices:

$$\underline{\underline{U}}^{-1} = \underline{\underline{W}}^{-1} + \underline{\underline{\Omega}} \qquad /V.1.25/$$

where matrix $\underline{\underline{W}}^{-1}$ is diagonal composed from the diagonal elements of $\underline{\underline{U}}^{-1}$ and $\underline{\underline{\Omega}}$ has zeros in the main diagonal while its off-diagonal elements are those of matrix $\underline{\underline{U}}^{-1}$. The elements of $\underline{\underline{W}}^{-1}$ are the reciprocals of the weights defined by eq. /V.1.4/. Now, the modified parameter estimates are solutions of the equation

$$\underline{G}(\underline{a}) = \underline{\underline{F}}^{T}\,\underline{\underline{W}}\underline{d} = 0 \qquad /V.1.26/$$

which is a modification of eq. /V.1.18/. By analogy with eq. /V.1.20/, we form matrix

$$\underline{\underline{M}}' = \underline{\underline{F}}^{T}\underline{\underline{W}}\underline{\underline{F}} \qquad /V.1.27/$$

and it can be simply derived that

$$\Delta\underline{a} = \underline{\underline{M}}'^{-1}\,\underline{\underline{F}}^{T}\,\underline{\underline{W}}(\Delta\underline{y}-\underline{\underline{\Gamma}}\Delta\underline{\mu}) \qquad /V.1.28/$$

instead of eq. /V.1.19/. Using eqs. /V.1.22/, the covariance matrix of $\underline{\tilde{a}}$ is obtained as

$$\frac{1}{\sigma^2}\langle \Delta\underline{a}\Delta\underline{a}^T\rangle = \underline{\underline{M}}'^{-1}\,\underline{\underline{F}}^T\,\underline{\underline{W}}(\underline{\underline{W}}_y^{-1}+\underline{\underline{\Gamma}}\underline{\underline{C}}\underline{\underline{\Gamma}})\underline{\underline{W}}\underline{\underline{F}}\underline{\underline{M}}'^{-1} = \underline{\underline{M}}'^{-1}+\underline{\underline{M}}'^{-1}\,\underline{\underline{F}}^T\underline{\underline{W}}\underline{\underline{\Omega}}\underline{\underline{W}}\underline{\underline{F}}\underline{\underline{M}}'^{-1}. \qquad /V.1.29/$$

It may be seen from this that a formal application of formula /II.1.13/ would be misleading if $\underline{\underline{\Omega}} \neq 0$ i.e. if the correction factors μ_i are correlated.

The importance of the additional term on the right hand side of eq. /V.1.29/ will be illustrated by a simple numerical example. Table V.1 presents exponentially decaying values. The statistical behaviour of these y_i is Poissonian. Suppose that the values belonging to x_i=1,4,7 are monitor counts and we are interested in extrapolating the other counts to x_i=0 relative to the extrapolation of the monitor counts. Since the monitor counts were selected from the same exponential as the other ones, the expectation of this value is 1.

Table V.1

x_i	y_i	x_i	y_i
1	9935	5	6952
2	9179	6	6607
3	8303	7	5859
4	7671		

The fitting function is very simple in this case: $g(z_i,\underline{a}) = a_1$ and we have only one parameter to determine. As stated above, the expected result is a_1=1. Considering the counts for x_1=2,3,5,6 as y_i , our formulae lead to

$$\underline{\underline{U}}^{-1} = \begin{bmatrix} 14099 & 3912 & 2208 & 846 \\ 3912 & 13136 & 3397 & 1553 \\ 2208 & 3397 & 10733 & 3007 \\ 846 & 1553 & 3007 & 10319 \end{bmatrix}$$

The numerical value of this matrix was given explicitely in order to show how large the off-diagonal elements can be. Now, the maximum likelihood method i.e. the solution of eq. /V.1.18/ and use of eq. /V.1.23/ with σ^2=1 yields $\tilde{a}_1$=1.00620 $\pm$ 0.009003 while the modified approach i.e. the solution of eq. /V.1.26/ and use of eq. /V.1.29/ yields $\tilde{a}_1$=0.99552 $\pm$ 0.009011.

As expected, the standard deviation is somewhat larger in the latter approach but the difference of the two standard deviations is hardly worth mentioning. This is, by the way, a good illustration of that it is not too dangerous to deviate a little from the maximum likelihood principle when it would lead to unjustified numerical complications /such as the handling of matrix $\underline{\underline{U}}$ would have been in our case/. There is, however, no excuse for ignoring the second term in the right hand side of eq. /V.1.29/ i.e. the term containing $\underline{\underline{\Omega}}$. If we neglect it, the resulting estimate is $\tilde{a}_1 = 0.99552 \pm 0.00711$. The standard deviation is underestimated by more than 20 %!

We conclude that eq. /V.1.26/ leads to fairly good parameter estimates but the off-diagonal elements of $\underline{\underline{\Omega}}$ may not be neglected in the error estimation. Some words are necessary concerning the computation of this additional term. The first problem is that the elements of $\underline{\underline{\Omega}}$ which are the off-diagonal elements of matrix $\underline{\underline{\Gamma}}\underline{\underline{C}}\underline{\underline{\Gamma}}$ /cf. eqs. /V.1.21/ and /V.1.25// depend on the parameter estimates /through $\underline{\underline{\Gamma}}$/. This difficulty may simply be overcome by setting $g(z_i, \tilde{\underline{a}}) \approx y_i^c$ what is a safe approximation for the purposes of the error estimation. Consequently, matrix $\underline{\underline{\Gamma}}\underline{\underline{C}}\underline{\underline{\Gamma}}$ may be computed once for ever before trying to solve eq. /V.1.26/ and it may be put on a magnetic tape. Then, after finding the parameter estimates, the content of the magnetic tape is read in only once and the errors are computed. All this requires hardly more than a few percents of the total computing time.

When we look at the procedure just described, we see that it is possible only if the primarily measured data are known. The reason is quite simple: if the corrections are carried out prior to the fitting and only the y_i^c are given as input to the fitting program, it is no more possible to calculate the elements of $\underline{\underline{\Omega}}$.

V.1.3 Correlated additive corrections. Constant background

In the previous section, multiplicative corrections were considered. The results can be directly transferred to the case of additive corrections. We reconsider here only the formulae of section V.1.2 i.e. when the off-diagonal elements are not taken into account in the parameter estimation. Now matrix $\underline{\underline{C}}$ stands for the covariance matrix of the background vector $\underline{\alpha}$ /with α_i as elements/ and the elements of $\underline{\underline{\Gamma}}$ are

$$\Gamma^{\alpha}_{ii} = \frac{\partial f(x_i, \underline{a})}{\partial \alpha_i} = \frac{1}{\nu_i} \, . \qquad /V.1.30/$$

With these changes, the formulae of section V.1.2 remain valid mutatis mutandis. This means that correlated additive corrections lead to an additional term in eq. /V.1.29/. Consequntly, the final expression for the covariance matrix of

the parameter estimates $\tilde{a}_k$ reads as

$$\frac{1}{\sigma^2} <\Delta\underline{a}\Delta\underline{a}^T> = \underline{\underline{M}}^{-1} + \underline{\underline{M}}^{-1} \underline{\underline{F}}^T \underline{\underline{W}} (\underline{\underline{\Omega}}_\mu+\underline{\underline{\Omega}}_\alpha) \underline{\underline{W}}\underline{\underline{F}}\underline{\underline{M}}^{-1} \qquad /V.1.31/$$

where the prime has been omitted in $\underline{\underline{M}}$. $\underline{\underline{\Omega}}_\mu$ and $\underline{\underline{\Omega}}_\alpha$ are the off-diagonal elements of matrices $\underline{\underline{\Gamma}}\underline{\underline{C}}\underline{\underline{\Gamma}}$ for $\underline{\mu}$ and $\underline{\alpha}$, respectively. $\underline{\underline{\Gamma}}$ is defined by eq. /V.1.30/ for $\underline{\alpha}$, and we remind that, for $\underline{\mu}$, it was defined as

$$\Gamma^{\mu}_{ii} = \frac{\partial f(x_i,\underline{a})}{\partial \mu_i} = \frac{g(z_i,\underline{a})}{\nu_i} \approx \frac{y^c_i}{\nu_i} \quad . \qquad /V.1.32/$$

The role of $\underline{\underline{\Omega}}_\mu$ was already illustrated by a numerical example. Now we illustrate the role of $\underline{\underline{\Omega}}_\alpha$ also by an example. The rather frequent case of a constant background will be considered i.e. when $\alpha_i=\alpha$ with a standard deviation of σ_α. Then

$$C^{\alpha}_{ii'} = \sigma^2_\alpha$$

and

$$\Omega^{\alpha}_{ii'} = (1-\delta_{ii'}) \frac{\sigma^2_\alpha}{\nu_i \nu_{i'}} \quad . \qquad /V.1.33/$$

As a numerical example, let us consider case 4 of Appendix 10. This is an exponential plus a background. We fit it to $g(z_i,\underline{a}) = a_1 e^{-a_2 z_i}$ and the background represented by $a_3=1000$ is assumed as measured separately, so that α is Poissonian with $<\alpha>=1000$. Now formula /V.1.31/ yields

$$\Delta\tilde{a}_1=114, \qquad \Delta\tilde{a}_2=0.00309$$

while neglecting $\underline{\underline{\Omega}}_\alpha$ would lead to

$$\Delta\tilde{a}_1=116, \qquad \Delta\tilde{a}_2=0.00324.$$

This shows that there is some effect in the errors /-2 % in $\Delta\tilde{a}_1$ and -5 % in $\Delta\tilde{a}_2$/ but it is not so large as the effect of $\underline{\underline{\Omega}}_\mu$.

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Our treatment of the problems of correlated corrections was sketchy. We ought to have revised the validity of all results of the previous chapters. This would be the subject of a separate paper. We must content ourselves with the short statement that mostof the results remain valid in a very good approximation since the correlated case can be reduced to the uncorrelated one.

The conclusions of the present section may be summarized as follows.

- It is immaterial whether the corrected values $/y_i^c/$ or the primary ones $/y_i/$ are used in the fitting until the corrections are statistically independent. The corresponding weights are given by eqs. /V.1.2/ and /V.1.4/.
- Only the primary data may be used in the fitting if the corrections are not statistically independent. Then the parameter estimation may be done as if they were be independent but the covariances have to be taken into account in the estimation of the parameters' standard deviations according to eq. /V.1.31/.

V.2 The normalization problem

V.2.1 Repeated measurements

One often encounters the problem of handling independent repetitions of the same measurement. Suppose for example that the measurement consists in the determination of the axial distribution within the reactor. The asymptotic part of the distribution curve has a cosine shape. Doing a fit to the function

$$f(x,\underline{a}) = a_1 \cos[a_2(x-a_3)],$$

we get the axial buckling as a_2 . If the measurement is repeated several times, the simplest - and most common - way of evaluation consists in repeating the fitting for each individual repetition and then averaging the resulting axial buckling values. /Here, the repetitions are understood as independent i.e. both irradiation and activity measurement are supposed to be repeated./ In addition to this, one is generally interested also in the shape of the distribution curve itself, especially in its transient part. In order to get such a curve from the individual repetitions of the measurement, they have to be normalized first and then some kind of average distribution curve may be drawn from them. It is clear that the reciprocals of the "amplitude" parameters a_1 are suitable normalization factors. The same procedure is applicable also when the shapes of the distribution curves obtained in the different repetitions are identical only in the asymptotic region but not necessarily so in the transient region. This is the case, for example, when the axial distribution is measured with different foil materials. Then, comparison of the normalized curves allows to study some spectral effects in the transient parts of the axial distributions.

This approach is theoretically simple and straightforward but not necessarily optimal. In the following, an other approach is described. Its

basic idea was first suggested to the author by J. Bardos. This idea proved to be very fruitful in practice because it turned out that quite a vast variety of problems may be treated on the basis of it. These are the problems in which one has to treat a couple of measured curves the shape of which can be described by the same function. The treatment of such measurements will be called here the normalization problem. Our approach will be formulated according to our introductory example but, later on, some further examples of applications will be cited demonstrating the possibilities of generalization. /See sections V.2.2 and V.2.3./

Let us suppose that our measured points $/x_i, y_i/$ can be divided into subsets R_j such that there exists a common shape function $\psi(x_i, \underline{a}_o)$ satisfying

$$\langle y_i \rangle = a_{j+m_o} \psi(x_i, \underline{a}_o) \quad \text{if} \quad i \in R_j \qquad /V.2.1/$$

$$j=1,2,\ldots,J$$

where m_o is the number of components of the common parameter vector $\underline{a}_o = (a_1, a_2, \ldots, a_{mo})$. Set R_j will be called runs. In case of the example cited above, $\psi(x, \underline{a}_o) = \cos[a_1(x-a_2)]$ and $m_o=2$ while parameter a_{j+2} is the amplitude parameter for run R_j so that the $1/a_{j+2}$ may be used as normalization factors. It is also clear that run R_j is identical with the distribution curve obtained in the j^{th} repetition of the measurement.

If eq. /V.2.1/ holds for the asymptotical regions of the measured curves, the evaluation may proceed according to the following fitting function:

$$f(x_i, \underline{a}) = a_{j+m_o} \psi(x_i, \underline{a}_o) \quad \text{if} \quad i \in R_j \qquad /V.2.2/$$

$$j=1,2,\ldots,J$$

where vector $\underline{a}$ is formed from the common parameters $\underline{a}_o$ and the amplitudes a_{j+m_o} $/j=1,2,\ldots,J/$. Then the total number of the unknown parameters is

$$m = m_o + J. \qquad /V.2.3/$$

Since we have found a suitable fitting function, the estimation of the unknown parameters may proceed from this point on exactly in the same way as described in the previous chapters. A necessary condition of that this normalization problem could be solved is that all runs contained at least one asymptotic point i.e. eq. /V.2.1/ should hold for at least one i in each of the runs.

As mentioned above, the ratios

$$y_i^n = \frac{y_i}{a_{j+m_o}} \qquad \text{if} \quad i \in R_j \qquad /V.2.4/$$

may be considered as points of the normalized distribution since they have expectations near $\psi(x_i, \underline{a}_o)$. It is important to note that the success of the normalization strongly depends on the choice of the shape function $\psi(x_i, \underline{a}_o)$. The statistical properties of the normalized values y_i^n can be easily derived using the general formulae of chapter II. The relevant formulae are summarized in Appendix 8.

The approach just described permits to estimate the normalization factors a_{j+m_o} and the common parameter vector $\underline{a}_o$ i.e. the same quantitites as by the approach in which the individual repetitions are evaluated separately and the resulting estimates are averaged. Therefore, some remarks are necessary as to why we prefer the use of the fitting function given in eq. /V.2.2/ to the other approach. The answer in short: this function leads to statistically better behaved estimates.

- The physical knowledge that the individual runs have the same shape is taken into account in the earliest possible stage of the evaluation by forcing the runs to have the same value for $\underline{a}_o$.
- If the runs are fitted separately, one has to average the individual results. As the number of runs is generally small /rarely more than 10/, this leads to the difficulties outlined in section V.3 in connection with the error estimation of the average. Such a problem does not even arise in our approach.
- In some cases /such as shown in Fig. V.1/, the separate fittings are often unsuccessful or at least unstable. At the same time, fitting according to eq. /V.2.2/ may be safe even in such cases.
- The chances for picking up defective points are much better when the runs are evaluated simultaneously. This is simply due to better statistical properties of the estimates.
- The most important advantage of the simultaneous fitting manifests itself in connection with the point drop technique. We have seen in section IV.4 that the error of second kind of the x^2 or Fisher tests results in a bias which is roughly proportional to the standard deviations of the parameter estimates. When the runs are fitted separately, the individual standard deviations will be relatively large and, consequently, so will be the individual biases. Now, when the average is calculated, the standard deviation of the mean will be about as small as the standard deviation of the estimate obtained in the simultaneous fitting but the

biases will not average out /just because they are systematic/. At the same time, the bias decreases parallelly with the standard deviation in the simultaneous fitting. We reach the conclusion that repeated measurements must be fitted simultaneously if the limits of the asymptotic region are determined by the point drop technique.

V.2.2 Furhter applications of the approach

Fitting functions like eq. /V.2.2/ are suitable when we have to treat distributions which may be internormalized by multiplication and the shape of which is known. This known shape $\psi(x_i,\underline{a}_o)$ may be given analytically /e.g. a cosine or a J_o Bessel-function/ with some unknown parameters to be fitted but it may be given numerically as well. In this latter case, only the amplitudes a_j are fitted /m_o=0/. This allows to normalize measurements to a directly computed distribution /see next section/.

Eq. /V.2.2/ is not the only possibility of treating data sets which bear something physically common. In order to illustrate the wide applicability of this approach, we present the following examples.

a/ Shifting of the runs:

$$f(x_i,\underline{a}) = \psi(x_i,\underline{a}_o) + a_{j+m_o} \quad \text{if } i\in R_j \qquad /V.2.5/$$

Such a fitting has always been used /already before the formulation of RFIT/ for the evaluation of temperature coefficient measurements when the reactivity was measured as a function of the temperature /x_i/ and it was necessary to make a stepwise move of a control rod from time to time. The runs may now be defined as the reactivity values belonging to the same control rod position. Function $\psi(x,\underline{a}_o)$ is usually a second order polinomial when the temperature range is not too wide $\psi(x,\underline{a}_o)=a_1x+a_2x^2$ and m_o=2.

b/ Both shifting and multiplication occur in the pulsed neutron source measurement of the subcritical reactivity when several detectors are used in different geometrical positions of the reactor. Let the runs be defined as the time analyser responses of the in ividual detectors. Then we have the fitting function

$$f(x_i,\underline{a}_o) = a_{2j+m_o}\,\psi(x_i,\underline{a}_o) + a_{2j+m_o-1} \quad \text{if} \quad i\in R_j \qquad /V.2.6/$$

where $\psi(x,\underline{a}_o)=e^{-a_1x}$ and m_o=1 for the fundamental mode. Taking into account that the point drop technique is the optimal means of finding the fundamental mode /which is now the asymptotic region/, only this fitting function ought to

be used for treating such measurements /see the remark at the end of section V.2.1/.

c/ For spectrum index measurements, this approach leads to a remarkably simple method of evaluation. Let us take the case of Pu/U as an example. The spectrum index is defined as

$$a_1 = \frac{A_{Pu}^{in}/A_u^{in}}{A_{Pu}^{th}/A_u^{th}} = \frac{A_{Pu}^{in}/A_{Pu}^{th}}{A_u^{in}/A_u^{th}} \qquad /V.2.7/$$

where A means foil activity, and superscripts "in" and "th" refer to irradiations in the investigated and the reference spectra, respectively. Generally, several repetitive irradiations are performed and, following each irradiation, the decaying activities of the foils are measured as functions of time.

Now the evaluation proceeds in the following way. For both Pu and U, the activites of the foils irradiated in the reference spectrum are considered as monitoring the decay of the foils irradiated in the investigated spectrum /see eqs. /V.18/ through /V.1.10//. Thus, we get decay correction factors μ_i^{Pu} and μ_i^{u} which will be simply proportional to the activities of the foils irradiated in the investigated spectrum the constants of proportionality being just A_{Pu}^{in}/A_{Pu}^{th} for Pu and A_u^{in}/A_u^{th} for U. If we denote the value of A_u^{in}/A_u^{th} for the j^{th} irradiation by a_{j+1}, then, according to eq. /V.2.7/, A_{Pu}^{in}/A_{Pu}^{th} for the same irradiation equals to $a_1\ a_{j+1}$.

Runs R_j are defined as follows. Let us consider the Pu activities for the first irradiation as R_1, the U activities for the same irradiation as R_2, the Pu activities for the second irradiation as R_3, the U activities for this irradiation as R_4 and so on. Then, together with the decay correction chosen above, the following fitting function describes the expectations of the measured activities

$$f(x_i,\underline{a}) = \begin{cases} a_1\ a_{j+1} & \text{if} \quad i \epsilon R_{2j-1} \\ a_{j+1} & \text{if} \quad i \epsilon R_{2j} \end{cases} \qquad /V.2.8/$$

Here, the number of unknown parameters in m=J/2+1.

By this approach, we solve three problems simultaneously in a statistically consistent way: carrying out the corrections, determining the spectum index, and synthesizing the results of the repetitions of the measurement.

This treatment may be applied to any spectrum index and disadvantage factor measurement when the decay is not assumed as exponential. If the decay

is exponential with a known decay constant, this treatment is still applicable but it leads to a slightly larger error of the spectrum index than the error resulting from the use of expoential decay correction factors. This is due to that formulae /V.1.8/ through /V.1.10/ do not take into account our knowledge of the value of the decay constants of the foils. An improved treatment may be derived in the following way.

d/ Suppose we have to determine the spectum index corresponding to isotopes "1" and "2":

$$a_1 = \frac{A_1^{in}/A_2^{in}}{A_1^{th}/A_2^{th}} \qquad /V.2.7a/$$

where the notations are analogous to eq. /V.2.7/. Let the numbers of irradiations in the investigated and the reference spectra be J^{in} and J^{th}, respectively. The activity values of both detectors 1 and 2 measured after each irradiation form a different run so that the total number of runs is $J=J^{in}+J^{th}$. For simplicity, let us assume that runs $j=1,2,\ldots J^{in}$ correspond to the investigated spectrum, while runs $j=J^{in}+1,\ldots,J^{in}+J^{th}$ to the reference spectrum. The decay corrected activity of detector 2 in run R_j is the unknown paramater a_{j+2} /j=1,2,...,J/. In addition to this, we have two run-independent parameters: $a_2=A_1^{th}/A_2^{th}$ and A_1^{in}/A_2^{in} which, according eq. /V.2.7a/, is equal to a_1a_2. Now the fitting function is

$$f(x_i,\underline{a}) = \begin{cases} a_{j+2} & \text{for detector 2} \quad \text{if } i\in R_j \\ a_2a_{j+2} & \text{for detector 1 and } j>J^{in} \quad \text{if } i\in R_j \\ a_1a_2a_{j+2} & \text{for detector 1 and } j\leq J^{in} \quad \text{if } i\in R_j \end{cases} \qquad /V.2.9/$$

and $m_o=2$, $m=J+2$.

It is an essential difference with respect to eq. /V.2.8/ that the numbers of irradiations in the reference and investigated spectra need not be the same for eq. /V.2.9/. As a matter of fact, approach c/ might also be reformulated in order to get rid of this restriction.

e/ In connection with axial distribution measurements, this technique was applied by J. Mikus to the solution of the following problem. In order to confine the fuel elements to well defined positions, an intermediate gridplate is mounted in the reactor approximately at midheight of the active length of the fuel rods. This perturbs the normal cosine shape of the axial distribution leading to a curve like that shown in Fig. III.4. At first glance, one is tempted to say that points near the perturbation should be dropped and a

cosine function could be fitted to the remaining points. It turned out that this procedure leads to too small axial buckling values because the effect of the gridplate is not restricted to its neighbourhood but it "pushes aside" the points lying on its left and right. Therefore, the following fitting function proved to work well:

$$f(x_i,\underline{a}) = \begin{cases} a_{2j+2}\cos[a_1(x_i-a_2)] & \text{if } i\in R_j,\ x_i<x_p \\ a_{2j+3}\cos[a_1(x_i-a_3)] & \text{if } i\in R_j,\ x_i>x_p \end{cases} \qquad /V.2.10/$$

$$m_o=3, \quad m=2J+3$$

where x_p is the coordinate of the perturbation.

V.2.3 Pure normalization

In the previous examples, shape function $\Psi(x_i,\underline{a})$ was known analytically and it always contained some unknown parameters /$\underline{a}_o$/ to be fitted. Therefore, the purpose of the evaluation was twofold: determination of $\underline{a}_o$ and normalization /i.e. determination of the run-dependent parameters a_{j+m_o}/. The case of a non-parametric shape function deserves a special attention.

Let us first consider the case when shape function $\Psi(x_i)$ is known. It makes no principal difference whether it is given by an analytical formula or it is given numerically. It may be result e.g. of a two-dimensional diffusion calculation /macrodistribution/ or of a THERMOS calculation /microdistribution/. Now the fitting function is very simple:

$$f(x_i,\underline{a}) = a_j\,\psi(x_i) \quad \text{if } i\in R_j \qquad /V.2.11/$$

$$m_o=0, \quad m=J$$

As the result of the fitting, we get only the normalization factors a_j allowing to internormalize the distributions measured in the individual runs. That is why such a fitting was called above "pure normalization". Once having determined parameters a_j , the normalization may be carried out in the following way. The corrected y_i^c values belonging to the same x_i are averaged first within each run and only then are the averages divided by factors a_j. The errors of the resulting normalized values may be computed on the basis of the formulae derived in Appendix 8. As the final step, for each x_i , we simply average the normalized values obtained for the individual runs R_j. We need not take into account any correlations in this step because, as it may be simply shown, the a_j are independent.

It is clear of course that the resulting normalized and averaged values depend on $\psi(x_i)$. For a $\psi(x_i)$ which is very inconsistent with the measured distributions, the success of this normalization procedure will be questionable especially when the different runs are only part overlapping i.e. the sets of x_i values belonging to different runs are not the same. A bad choice of $\psi(x_i)$ leads to an overestimation of the errors of the normalized values. Consequently, the direct comparison of the normalized and theoretical distributions can not be recommended.

Now, the following justified question may be raised: why to formulate a simple problem like normalization as a complicated fitting problem? Indeed, the corrections may be carried out by hand /or by small programs adapted to the measurement at hand/ and then the normalization factors a_j may be determined e.g. by comparing the areas under the measured and theoretical curves. We still recommend our formulation for the following reasons:

- The experimental data are supposed to be available on paper or magnetic tapes. This allows to do a computerized data reduction. If a general fitting program is available, there is no reason why not to do the data reduction by using this.
- A general fitting program like RFIT offers additional services besides the data reduction such as searching defective points and pointwise comparison of the measured and theoretical values /see section III.2/, the point drop technique /see chapter IV/ etc.
- A goodness of fit test may be based on the resulting value of Q_{min} /see section V.2.4/.

It is a frequent case that we do not have any given $\psi(x_i)$ but we still want to obtain a sound normalized and averaged distribution curve. In other words, not only the normalization parameters a_j but also the $\psi(x_i)$ values are unknown. Let us denote by r_I /I=1,2,...,N/ the "foil positions" i.e. all the different values which occur among the x_i taking into account all runs. For the correspondig $\psi(r_I)$, we introduce the notation ψ_I. Now we have the fitting function

$$f(x_i,\underline{a}) = a_j \psi_{I_i} \qquad \text{if} \quad i \in R_j \qquad \text{/V.2.12/}$$

$$m=J+N$$

where I_i is such a subscript for which $r_{I_i}=x_i$. The compoents of vector $\underline{a}$ are the following: the first J are the a_j /j=1,2,...J/ while

$$a_{j+I} = \psi_I \ . \qquad \text{/V.2.13/}$$

In practical cases, this fitting function provides only a formal solution. Number N of the positions may be as large as 100 so that the general fitting procedure would involve the inversion of about 100 by 100 matrices. This is not only time consuming but sometimes also numerically unstable. Therefore, we need a special solution. Let us write down explicitely the sum of squares to be minimized taking into account the corrections, too:

$$Q = \sum_{j=1}^{J} \sum_{i \in R_j} W_i (y_i - a_j \psi_{I_i} \mu_i - \alpha_i)^2 \quad . \qquad /V.2.14/$$

Differentiating Q with respect to a_j and ψ_I , we get after some algebra that

$$\tilde{a}_j = \frac{\sum_{i \in R_j} W_i (y_i - \alpha_i) \tilde{\psi}_{I_i} \mu_i}{\sum_{i \in R_j} W_i (\tilde{\psi}_{I_i} \mu_i)^2} \quad , \quad j=1,2,\ldots,J \qquad /V.2.15/$$

$$\tilde{\psi}_I = \frac{\sum_{j=1}^{J} \sum_{\substack{i \in R_j \\ x_i = r_I}} W_i (y_i - \alpha_i) \tilde{a}_j \mu_i}{\sum_{j=1}^{J} \sum_{\substack{i \in R_j \\ x_i = r_I}} W_i (\tilde{a}_j \mu_i)^2} \quad , I=1,2,\ldots,N \qquad /V.2.16/$$

This set of equations may be solved by iteration as described in Appendix 9. It is shown there that one of the unknowns or a linear combination of the ψ_I values might be fixed to an arbitrary value.

By practical difficulties, we were forced to abandon the general Newton iteration described in section I.3 for solving the least squares equations, cosequently, the inverse of matrix $\underline{\underline{M}}$ defined by eq. /I.3.5/ is not available for the estimation of the errors /cf. eq. /II.1.13//. We need therefore some alternative error formula. Since the ultimate purpose of the evaluation in this case is the determination of the distribution i.e. of the ψ_I , we restrict ourselves to the estimation of their errors. Parameters a_j are only auxiliary quantities and, as such, they play only a secondary role.

The estimation of the error of $\tilde{\psi}_I$ is much simpler if the whole problem is reformulated in terms of the corrected values y_i^c . As shown in section V.1, we have right to do that. Starting from eq. /V.1.5/ instead of eq. /V.2.14/ which now reads as

$$Q = \sum_{j=1}^{J} \sum_{i \epsilon R_j} w_i^c (y_i^c - a_j \psi_{I_i})^2 \qquad /V.2.17/$$

where

$$\langle (y_i^c)^2 \rangle = \frac{\sigma^2}{w_i^c} , \qquad /V.2.18/$$

This leads to

$$\tilde{\psi}_I = \frac{\sum_{j=1}^{J} \sum_{\substack{i \epsilon R_j \\ x_i = r_I}} w_i^c \, y_i^c \, \tilde{a}_j}{\sum_{j=1}^{J} \sum_{\substack{i \epsilon R_j \\ x_i = r_I}} w_i^c \, \tilde{a}_j^2} \qquad /V.2.19/$$

Here, y_i^c and $\tilde{a}_j$ are both random variables but the standard deviations of $\tilde{a}_j$ is generally by an order of magnitude less than that of y_i^c . Therefore, $\tilde{a}_j$ may be considered as a constant. In this approximation, it is straightforward to show that

$$\langle (\Delta \psi_I)^2 \rangle = \frac{\sigma^2}{\sum_{j=1}^{J} a_j^2 \sum_{\substack{i \epsilon R_j \\ x_i = r_I}} w_i^c} \qquad /V.2.20/$$

This formula applies only if the corrections are uncorrelated. In case of correlated corrections, the error formula is analogous and may be also simply derived on the basis of eq. /V.2.19/.

When the decay correction factors μ_{di} are determined from monitor counts, the monitor may also be considered as a position of the distribution ψ_I. Then all $(y_i - \alpha_i)$ have to be substituted by μ_{di} as the corresponding measured values.

V.2.4 A goodness-of-fit test in case of pure normalization

In the previous section, two methods were described. The method based on the fitting function /V.2.12/ is almost free from assumptions. Only the existence of a common shape function ψ_I is assumed. This may be warranted if only such measurements are internormalized which were performed really for the same reactor state by the same experimental technique. Of course, if the existence of the common shape function may be assumed only for a subset of positions, this subset can be found as the asymptotic region by the point drop technique described in chapter IV.

With such an assumption, we may write according to eq. /II.3.1/ that

$$Q_{min} = \sigma^2 \chi^2_{n-J-N} \qquad /V.2.21/$$

where n is the total number of points taken into account in eq. /V.2.14/. This allows a sound estimation of σ^2 by formula /II.3.2/.

A similar statement is generally not possible for fitting function /V.2.11/ because the purpose of the normalization is just to check the agreement of the theoretical distribution $\psi(x_i)$ with the measured values. Consequently, it may not be assumed that eq. /II.3.1/ holds for the resulting Q_{min} . As mentioned in the previous section, this Q_{min} may be used for checking the goodness of fit if σ^2 is known. These two approaches described for pure normalization can be combined for the realization of this.

Let us suppose that we have made a normalization according to fitting function /V.2.12/ resulting in the normalized distribution $\tilde{\psi}_I$. Variances $\langle(\Delta\psi_I)^2\rangle$ are written as

$$\langle(\Delta\psi_I)^2\rangle = \frac{\sigma^2}{W_I} \qquad /V.2.22/$$

where, according to eq. /V.2.20/,

$$W_I = \sum_{j=1}^{J} \tilde{a}_j^2 \sum_{\substack{i \in R_j \\ x_i = r_I}} w_i^c \; . \qquad /V.2.23/$$

Let us denote the theoretical distribution by $\psi(r_I)$. This is assumed to be given for each position r_I. It is sufficient to compare this distribution to $\tilde{\psi}_I$ on the basis of a normalization according to eq. /V.2.11/ i.e.

$$f(r_I, a_1) = a_1 \psi(r_I). \qquad /V.2.24/$$

The sum of squares to be minimized now reads as

$$Q' = \sum_{I=1}^{N} W_I (\tilde{\psi}_I - a_1 \psi(r_I))^2. \qquad /V.2.25/$$

The solution for a_1 is now trivial:

$$a_1 = \frac{\sum_{I=1}^{N} W_I \tilde{\psi}_I \; \psi(r_I)}{\sum_{I=1}^{N} W_I \; [\psi(r_I)]^2} \qquad /V.2.26/$$

and its variance is

$$\langle(\Delta a_1)^2\rangle = \frac{\sigma^2}{\sum_{I=1}^{N} W_I \left[\psi(r_I)\right]^2} \quad . \qquad /V.2.27/$$

If the theoretical distribution is in agreement with the given experiment, i.e. when

$$\langle\tilde{\psi}_I\rangle = \psi(r_I) \qquad /V.2.28/$$

for all positions r_I, eq. /II.3.1/ holds, consequently,

$$Q'_{min} = \sigma^2 \chi^2_{N-1} \quad . \qquad /V.2.29/$$

From these χ^2 variables, a Fisher-fraction can be formed. We have shown in section II.5 that Q_{min} and the parameter estimates are statistically independent. In our present case, this means that Q_{min} and all $\tilde{\psi}_I$ are statistically independent. This assures that so are Q_{min} and Q'_{min} the latter being a function of $\tilde{\psi}_I$ as eqs. /V.2.25/ and /V.2.26/ show. We conclude now that

$$f_{N-1,n-J-N} = \frac{Q'_{min}/(N-1)}{Q_{min}/(n-J-N)} = \frac{\chi^2_{N-1}/(N-1)}{\chi^2_{n-J-N}/(n-J-N)} \qquad /V.2.30/$$

is a random variable distributed according to Fisher's distribution. The goodness-of-fit test is then carried out in the usual way: if

$$\frac{Q'_{min}/(N-1)}{Q_m/(n-J-N)} < \gamma_f \quad , \qquad /V.2.31/$$

we decide for the agreement of theory and experiment, while for the disagreement in the opposite case. Here, γ_f is the quantile of the Fisher distribution with indices /N-1/ and /n-J-N/.

Besides this Fisher-test, the pointwise Student test may also be performed on the basis of the comparison of $\tilde{\psi}_I$ and $\tilde{a}_1\psi(r_I)$. In this case, the Student test can be formulated in a more advantageous way than in chapter III. Namely, according to eq. /III.2.8/, Q'_{min} ought to be used for this purpose. The main goal of this fitting is, however, just the test of the goodness-of-fit, consequently, it is not a good policy to rely on that Q'_{min} is $\sigma^2\chi^2_{N-1}$. It is more advantageous to build the test on Q_{min}, for which eq. /V.2.21/ surely holds /unless distribution $\tilde{\psi}_I$ was composed from incompatible measurements.. Now, eq. /III.2.8/ results in the fractions

$$t_I = \frac{(\tilde{\psi}_I - \tilde{a}_1 \psi(r_I)) \sqrt{W_I}}{\sqrt{\frac{Q_{min}}{n-J-N} \left(1 - \frac{W_I [\psi(r_I)]^2}{\sum_{I'=1}^{N} W_{I'} [\psi(r_{I'})]^2}\right)}} \qquad /V.2.32/$$

for I=1,2...,N which are Student variables with a number of degrees of freedom equal to /n-J-N/.

V.2.5 Numerical examples

Fig. V.1 shows case 11 in which the same cosine distribution was measured in three pieces. That is why they have different amplitudes. A fitting according to eq. /V.2.2/ with $\psi(x, \underline{a}_o) = \cos[a_1(x-a_2)]$ and J=3 leads to $\tilde{a}_1 = (1.985 \pm 0.007) \cdot 10^{-2}$. Fig V.1a shows the pieces /which are now runs R_1, R_2, R_3/ as they were measured while Fig. V.1b shows the y_i^n values normalized according to eq. /V.2.4/. We see that this way of evaluation solves both the estimation of the common parameters a_1 and a_2 and the normalization. If we try to fit function $f(x,\underline{a}) = a_1 \cos[a_2(x-a_3)]$ to these pieces separately, the results are generally rather unstable, especially for R_3.

As the next example, let us return to cases 1, 2, and 3 treated in section II.2. The results of the separate fittings were presented in Table II.1. We have seen that the evaluation of case 3 is rather uncertain due to its poor statistical accuracy. We give here the results of the simultaneous fitting according to eq. /V.2.2/ when each case represents a run. The buckling parameter /a_1 here, a_2 in Table II.1/: $\tilde{a}_1 = (2.02089 \pm 0.01830) \cdot 10^{-2}$ ($\delta a_1 = 5.9) \cdot 10^{-6}$; the position of the maximum /a_2 here, a_3 in the table/: $\tilde{a}_2 = 30.4791 \pm 0.3972$ ($\delta a_2 = 0.017$). The weighted average of the $\tilde{a}_2$ values given in Table II.1 is $(2.02110 \pm 0.01761) \cdot 10^{-2}$ /the average of the bias: $1.7 \cdot 10^{-5}$/; the same for $\tilde{a}_3$ is 30.5434 ± 0.3815 /with an average of the bias: 0.040/. We gave these values with an unusually large number of digits in order to show that the results of the simultaneous fitting practically correspond to a weighted average as far as the common parameters are concerned. It follows from this that, due to its low weight, case 3 can not influence the final results significantly. From the point of view of the common parameters, it may even be left out of consideration.

The simultaneous fitting, however, results in very good estimates for the amplitudes of even the very inaccurate runs. Here are the obtained amplitudes with the biases in parantheses:

case 1:	9986.82 ± 17.76	(-0.41)
case 2:	992.30 ± 4.35	(-0.040)
case 3:	98.63 ± 1.32	(-0.004)

When these amplitudes are compared to those given in Table II.1, it can be seen that both the standard deviations and the biases are sensibly reduced for cases 2 and 3. This is especially striking for case 3 which seemed to be hopeless on the basis of the separate fitting. It is also interesting to note that the error of the amplitude for case 1 slightly increased with respect to Table II.1. Of course, this does not matter but one must be aware of that this did not happen by chance. Heuristically, this may be explained by that part of the information content of case 1 has been spent on improving the estimation of the amplitudes of cases 2 and 3.

Finally, we show in Fig. V.2 how the point drop technique works in case of simultaneous fitting. In section IV.6, we treated cases 7 and 9 separately. They have been evaluated according to eq. /V.2.2/ with $\psi(x,\underline{a}_o) = \cos[a_1(x-a_2)]$. Runs R_1 and R_2 were cases 7 and 9, respectively. The point drop limits were defined exactly in the same way as in the individual fittings i.e. 2 points were dropped from both runs in each step. The plots in Fig. V.2 are analogous to the plots in Figs. IV.7 or IV.11. The results were the following. The φ-test accepted step 12 as asymptotic while the Fisher-test for parameter a_1 recommends only step 14. As we settled in chapter IV, we rely on this last recommendation. The estimate from step 14 for the buckling parameter is $\tilde{a}_1 = (1.999 \pm 0.010) \cdot 10^{-2}$. The upper bound for the systematic error is $\delta p_o = 6.8 \cdot 10^{-5}$. The limit of the asymptotic region in step 14 is $x_i \triangleq 69$. If we compare this with the conclusion of section IV.6 where $x_i \triangleq 79$ has been found for both cases as the asymptotic region, we see that the simultaneous fitting narrowed it down.

This example is typical. When we studied the results of the individual fittings, the asymptotic region $x_i \triangleq 79$ seemed to be all right. Now we learn that the interval $69 < x_i \triangleq 79$ contains transient points with a high probability. Indeed, the pointwise Student-test declares all points of case 7 too high in this region. For case 9 where the transient term is smaller, these points are accepted by the Student-test. We conclude now that the buckling estimate obtained from the separate fitting of case 7 (0.01979 ± 0.00011) contains a sytematic error, cosequently, this estimate is significantly too low.

The main points can summarized as follows. First, it is always advisable to perform a final simultaneous fitting when we have several repetitions of the same measurement because this allows to make much more safe conclusions. Second, the statistical analysis made on the basis of the simultaneous fitting can give useful additional information concerning the individual measurements. In the example studied above, we had no idea without the simultaneous fitting how good the asymptotic region $x_i \triangleq 79$ really was.

V.3 Averaging

The averaging is an important special case of the fitting problem. It corresponds to the fitting function

$$f(x_i,a) = a \; , \qquad m=1 \; . \qquad /V.3.1/$$

All the considerations made and all the results obtained in the previous chapters are directly applicable but some aspects are worth-while to study in more detail.

The least squares method gives the following trivial estimate for the mean of the quantities y_i to be averaged:

$$\tilde{a} = \bar{y} = \frac{\sum_{i=1}^{n} W_i y_i}{\sum_{i=1}^{n} W_i} \qquad /V.3.2/$$

while formula /II.1.13/ is now reduced to

$$\Delta\tilde{a} = \sqrt{\frac{\sigma^2}{\sum_{i=1}^{n} W_i}} \; . \qquad /V.3.3/$$

σ^2 is estimated as before by formula /II.3.2/ yielding

$$\tilde{\sigma}^2 = \frac{Q_{min}}{n-1} \; . \qquad /V.3.4/$$

When number n of the averaged values is large, one can stop at this point. Indeed, formulae /V.3.3/ and /V.3.4/ allow to obtain a good error estimation and the results of chapter III offer sound confidence intervals for both $\tilde{a}$ and y_i. Things are much less favourable when n is small. Therefore, we study the difficulties arising from the smallness of n.

Let us consider a case when we average 4 Gaussian quantities y_i /i=1,2,3,4/ having the same error Δy. Eq. /V.3.3/ yields for the error of the average:

$$\Delta\tilde{a} = \sigma \, \frac{\Delta y}{2}$$

where σ^2 is estimated using eq. /V.3.4/. If we suppose that Δ_y is the real standard deviation of y_i, $\tilde{\sigma}^2$ will be approximately equal to 1 i.e. $\Delta\tilde{a} \approx \Delta y/2$. Now, we form a confidence interval for a using eq. /III.1.4/. Its half width is $\gamma\Delta\tilde{a} = \gamma\Delta y/2$ which, for ε=0.01, is equal to 2.92 Δy /see Table A.1/. It is

interesting to compare this to the confidence interval which could have been formed without averaging i.e. using only one out of the y_i , say y_1 . Since y_1 is Gaussian, the half width of this interval is only 2.58 Δy . We got the surprising result that the confidence interval of the average is broader than that of the averaged quantities. In other words, we lost information by averaging what seems to be a nonsense. The reason of this loss of information is clear: the usage of eq. /V.3.4/ results in a rather uncertain error estimation. That is why quantile γ is as high as 5.84 in this case.

Now, the natural question arises whether we are really obliged to use formula /V.3.4/. As a matter of fact, we are not. In order to make this statement clear, let us suppose that we perform axial distribution measurements and to each measured curve a cosine is fitted separately yielding estimate y_i of the axial buckling for the i^{th} repetition of the measurement. Average $\tilde{a}$ given by eq. /V.3.2/ is also an estimate of the axial buckling. The error of each y_i is also estimated by the fitting program. These error estimates may be supposed to be correct if the measurement and the studied reactor configuration are reproducible. Then, we may set $\sigma^2=1$ with assurance and we could omit the usage of eq. /V.3.4/. This implies that Gaussian quantiles may be accepted when forming confidence intervals for $\tilde{a}$. This assures that the confidence interval for the average is always narrower than that for the averaged quantities.

When, in turn, the measurement and/or the studied reactor configuration may not be supposed to be reproducible, the y_i values will show larger fluctuations than expected on the basis of their errors as estimated by the fitting program. Therefore, we must assume the existence of an additional component in their errors and this is just what is taken into account by σ^2. Consequently, σ^2 has to be estimated by eq. /V.3.4/. We have seen above that this is rather uncertain if n i.e. the number of repetitions is small. The fact is that, when we decide to repeat our measurement only a small number of times, we tacitely assume the reproducibility. Consequently, it is not advisable to make such a decision if we do not control all parameters of the measurement.

All these problems do not arise if the evaluation is performed by the method described in section V.2. The reason of this is that σ^2 is estimated with a much larger number of degrees of freedom.

When n is small, condition /III.2.10/ which was formulated for rejecting eventual defective points is to be used with care. Let us take again the case n=4 as an example. The t_i fraction defined by eq. /III.2.8/ is bounded by $\sqrt{3}$ = 1.732 according to formula /III.2.12/. Table A.1 gives γ' = 1.715 for this n and for ε=0.01. This means that y_i is rejected as defective if the corresponding t_i is such that $|t_i|>1.715$. We see that the critical region /the interval in which the value is rejected/ is rather narrow: from 1.715 to 1.732. This means that even very bad y_i values lead to t_i fractions which

are hardly above quantile γ' . If one forgets about this consequence of the smallness of n, a t_i=1.725, for example, seems to be a borderline case and one is tempted to meditate whether it is really necessary to reject the corresponding y_i . In fact, such a t_i is caused by a fairly deviating y_i . When t_i' is calculated according to eq. /III.2.9/, we get that t_i'=15.9 which is to be compared with γ=9.93 /see Table A.1/. On the basis of this comparison, one has much less confidence in value y_i.

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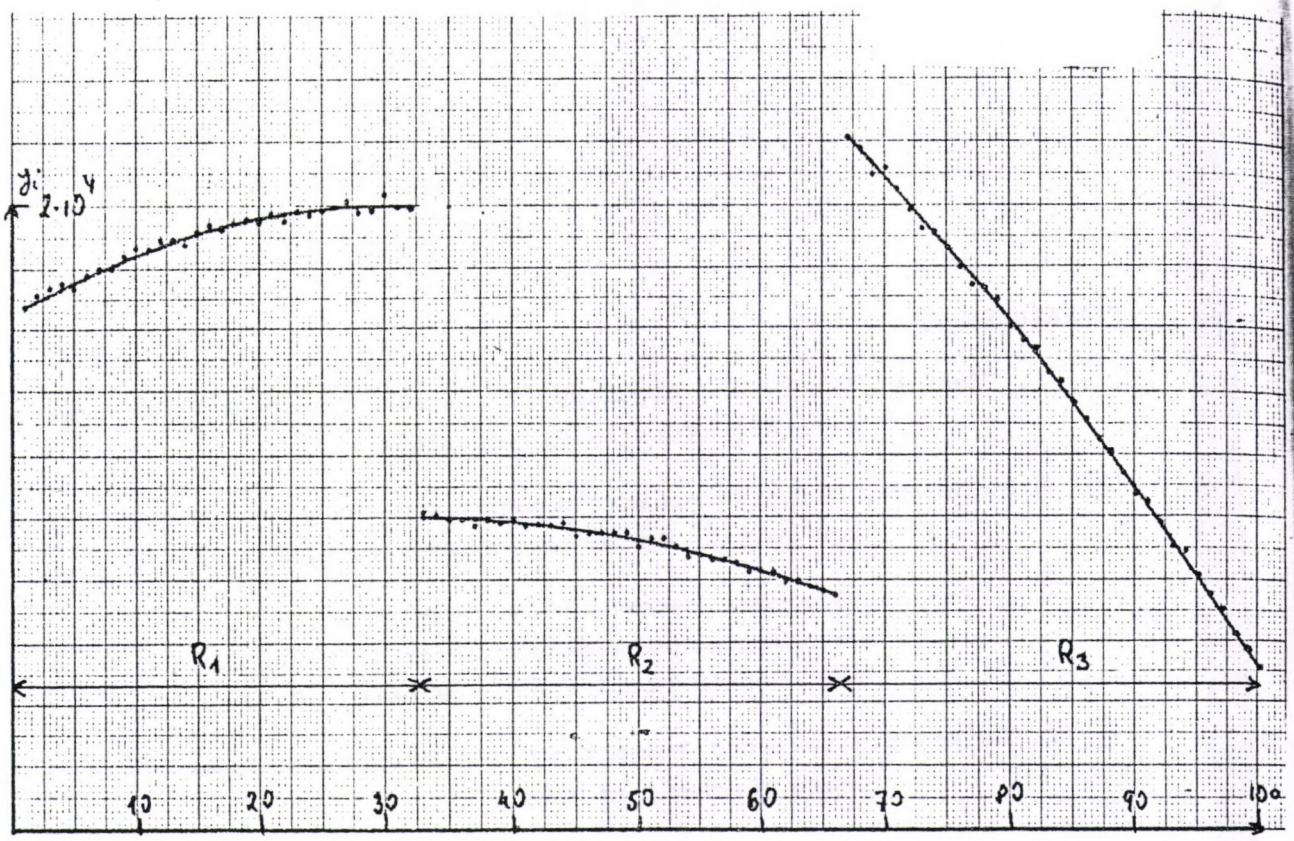

Fig. V. 1a

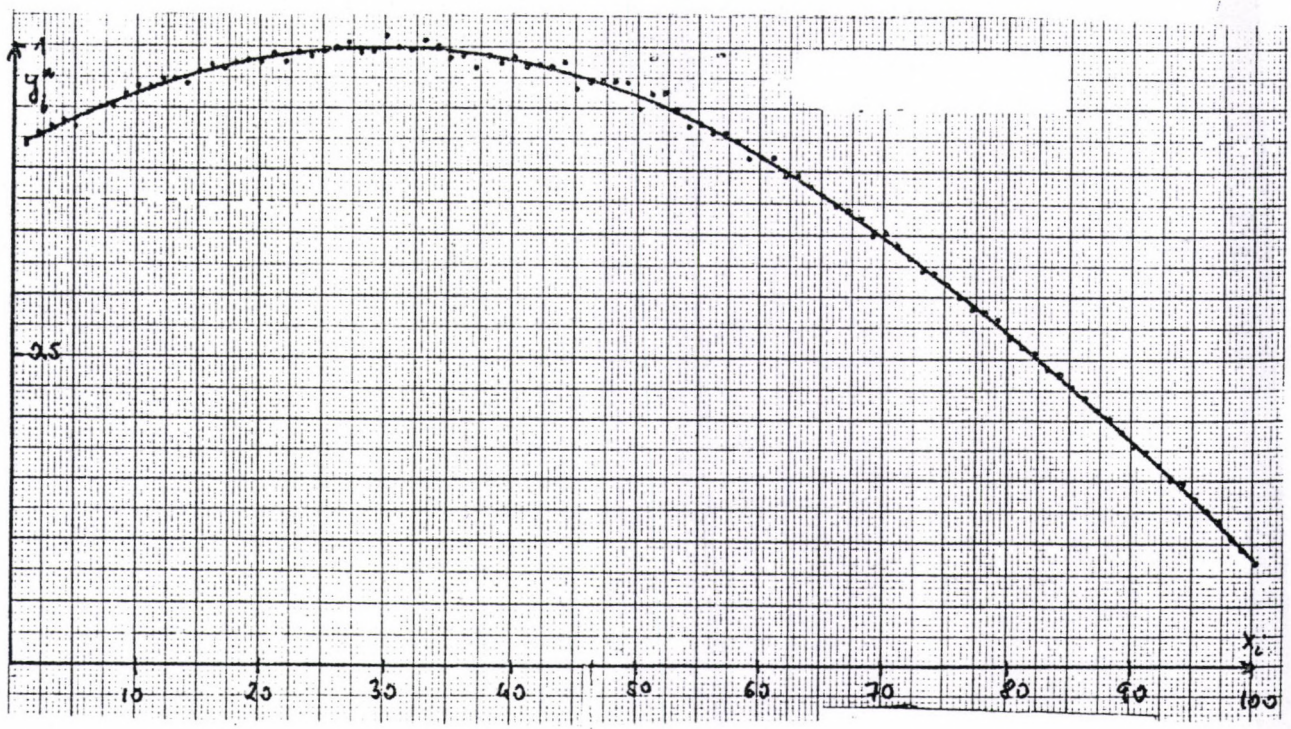

Fig. V. 1b

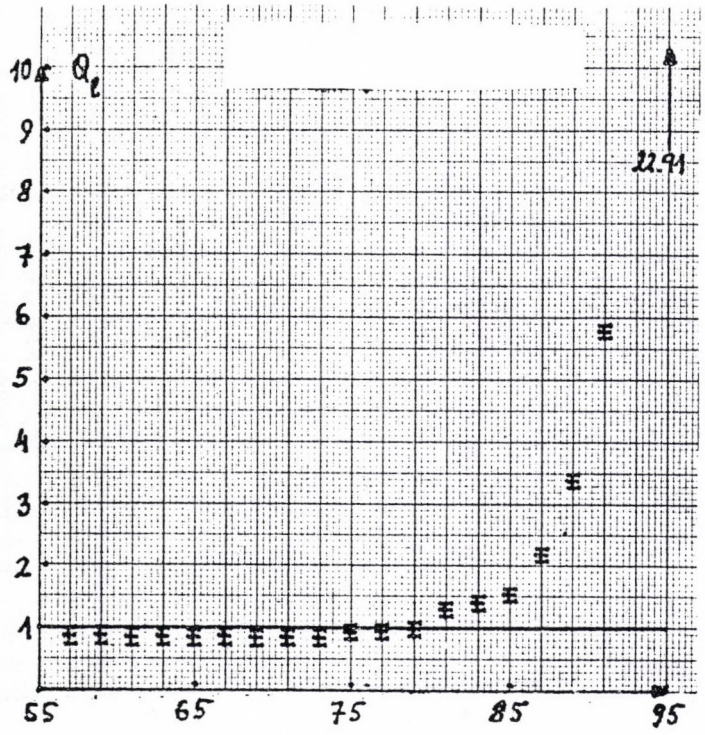

Fig. V. 2a

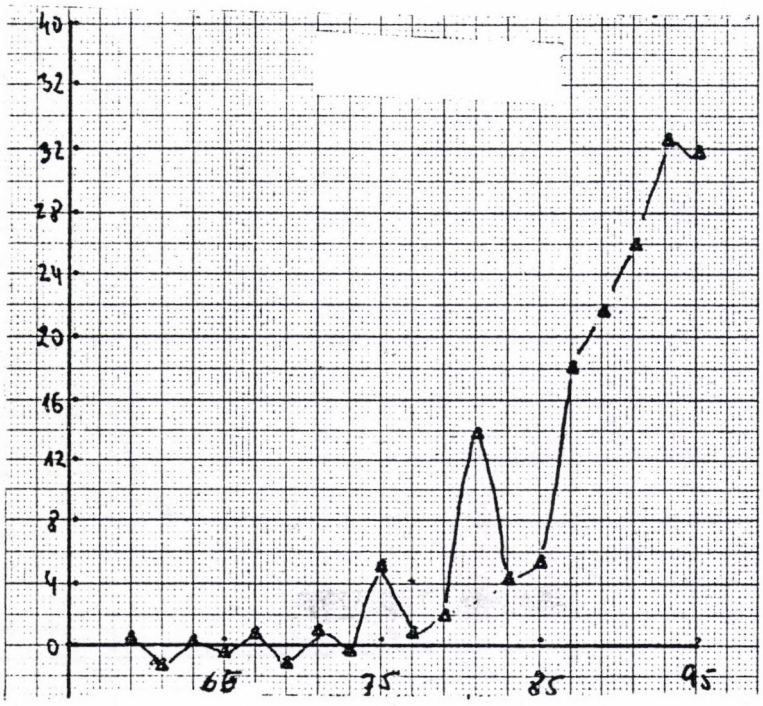

Fig. V. 2b

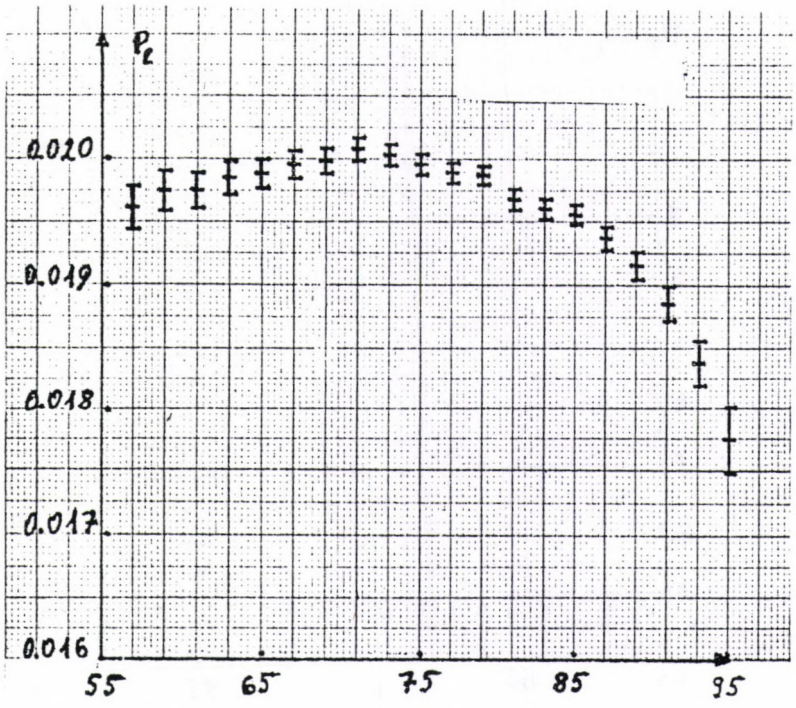

Fig. V. 2c

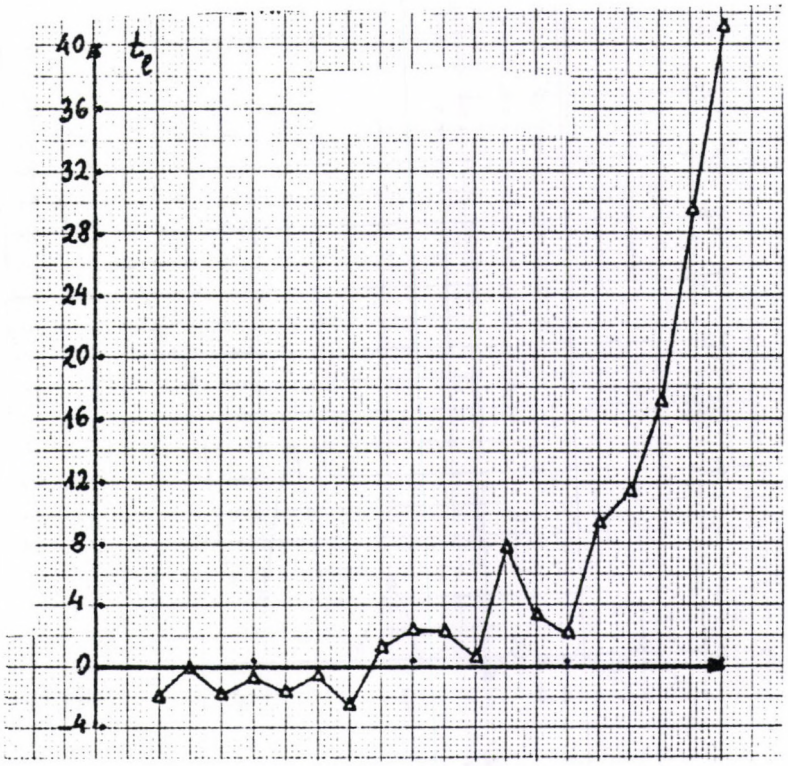

Fig. V. 2d

APPENDIX 1.

PROOF OF EQS. /III.2.9/ AND /III.2.11/

Eqs. /III.2.9/ and /III.2.11/ will be proved neglecting the bias. Let us denote the i^{th} row of matrix $\underline{\underline{F}}$ by $\underline{f}_i^T$. From eq. /II.4.2/, we have that

$$\tilde{y}_i = f(x_i,\underline{a}) + \underline{f}_i^T\Delta\underline{a} = f(x_i,\underline{a}) + \Delta\underline{a}^T\underline{f}_i \qquad /A.1.1/$$

and the minimum of the sum of squares may be written as

$$Q = \sum_{j=1}^{n} w_j(\Delta y_j - \Delta\underline{a}^T\underline{f}_j)^2 \qquad /A.1.2/$$

where, for the sake of simplicity, Q was written instead of Q_{min}. Eq. /III.2.7/ may be rewritten as

$$<(y_i - \tilde{y}_i)^2> = \frac{\sigma^2}{w_i^*} \qquad /A.1.3a/$$

where

$$\frac{1}{w_i^*} = \frac{1}{w_i} - \underline{f}_i^T\,\underline{\underline{M}}^{-1}\,\underline{f}_i. \qquad /A.1.3b/$$

We shall need more explicite expressions for $\underline{\underline{M}}$ and $\Delta\underline{a}$ than eqs. /II.1.4/ and /II.1.12/, respectively:

$$\underline{\underline{M}} = \underline{\underline{F}}^T\underline{\underline{W}}\underline{\underline{F}} = \sum_{j=1}^{n} w_j\underline{f}_j\underline{f}_j^T \qquad /A.1.4/$$

and

$$\Delta\underline{a} = \underline{\underline{M}}^{-1}\,\underline{\underline{F}}^T\underline{\underline{W}}\Delta\underline{y} = \underline{\underline{M}}^{-1}\sum_{j=1}^{n} w_j\Delta y_j\underline{f}_j. \qquad /A.1.5/$$

Leave now y_i out from the fit. Then matrix $\underline{\underline{M}}$ goes over in

$$\underline{\underline{M}}_i = \sum_{j\neq i} w_j\underline{f}_j\underline{f}_j^T = \underline{\underline{M}} - w_i\underline{f}_i\underline{f}_i^T \qquad /A.1.6/$$

and $\Delta\underline{a}$ goes over in

$$\Delta\underline{a}_i = \underline{\underline{M}}_i^{-1} \sum_{j\neq i} w_j \Delta y_j \underline{f}_j = \underline{\underline{M}}_i^{-1} \left(\underline{\underline{M}}\Delta\underline{a} - w_i \Delta y_i \underline{f}_i\right) \qquad /A.1.7/$$

as it may be shown using eqs. /A.1.4/ and /A.1.5/. The sum of squares Q goes over in Q_i which is equal to

$$Q_i = \sum_{j\neq i} w_j (\Delta y_j - \Delta\underline{a}_i^T \underline{f}_j)^2 = \sigma^2 \chi^2_{n-m-1} \qquad /A.1.8/$$

if eq. /II.3.1/ is also taken into account. We know from section II.5 that Q_i is independent of $\Delta\underline{a}_i$. It is evidently independent of y_i and so of $\Delta\underline{a}$, too, the latter being a linear combination of Δy_i and $\Delta\underline{a}_i$ /see eq. /A.1.7//. Furthermore, $(y_i - \tilde{y}_i)$ is a linear combination of y_i and $\Delta\underline{a}$, therefore, we conclude that Q_i and $(y_i - \tilde{y}_i)$ are independent.

When point y_i is left out, the expression

$$f(x_i, \underline{a}) + \Delta\underline{a}_i^T \underline{f}_i$$

will play the role of $\tilde{y}_i$ /cf. eq. /A.1.1// and, according to eq. /III.2.3/, the Student-fraction t_i' is given by the formula

$$t_i' = \frac{(\Delta y_i - \Delta\underline{a}_i^T \underline{f}_i)\sqrt{w_i^{**}}}{\sqrt{\frac{Q_i}{n-m-1}}} \qquad /A.1.9/$$

where

$$\frac{1}{w_i^{**}} = \frac{1}{w_i} + \underline{f}_i^T \underline{\underline{M}}_i^{-1} \underline{f}_i . \qquad /A.1.10/$$

Eq. /III.2.8/ is rewritten in the notations of the present Appendix as

$$t_i = \frac{(y_i - \tilde{y}_i)\sqrt{w_i^*}}{\sqrt{\frac{Q}{n-m}}} = \frac{(\Delta y_i - \Delta\underline{a}^T \underline{f}_i)\sqrt{w_i^*}}{\sqrt{\frac{Q}{n-m}}} \qquad /A.1.11/$$

The connection between t_i and t_i' may be found on the basis of the following relationships:

$$w_i^* w_i^{**} = w_i^2 , \qquad /A.1.12/$$

$$Q_i = Q\left(1 - \frac{t_i^2}{n-m}\right) , \qquad /A.1.13/$$

and

$$(\Delta y_i - \Delta\underline{a}_i^T f_i)\sqrt{w_i^{**}} = t_i \sqrt{\frac{Q}{n-m}} . \qquad /A.1.14/$$

In fact, putting these expressions in eq. /A.1.9/, we get the desired result:

$$t_i' = \frac{t_i \sqrt{\frac{Q}{n-m}}}{\sqrt{\frac{Q}{n-m-1}\left(1 - \frac{t_i^2}{n-m}\right)}} = \frac{t_i}{\sqrt{1 - \frac{t_i^2 - 1}{n-m-1}}} \qquad /A.1.15/$$

as stated by eq. /III.2.9/. The second equation, i.e. eq. /III.2.11/ is now a direct consequence of eq. /A.1.15/. The unequality $|t_i'| < \gamma$ may be written as

$$t_i'^2 < \gamma^2$$

which is evidently equivalent to

$$t_i^2 < \frac{\gamma^2}{1 + \frac{\gamma^2 - 1}{n-m}} = \gamma'^2 \qquad /A.1.16/$$

which proves eq. /III.2.11/.

To complete the present Appendix, we have the proves of eqs /A.1.12/ to /A.1.14/ left. From eqs. /A.1.3b/ and /A.1.10/, we have that

$$\frac{W_i^2}{W_i^* W_i^{**}} = (1 - W_i \underline{f}_i^T \underline{\underline{M}}^{-1} \underline{f}_i)(1 + W_i \underline{f}_i^T \underline{\underline{M}}_i^{-1} \underline{f}_i) = 1 + W_i \underline{f}_i^T \underline{\underline{M}}_i^{-1} \underline{f}_i - W_i \underline{f}_i^T \underline{\underline{M}}^{-1} \underline{f}_i - W_i^2 \underline{f}_i^T \underline{\underline{M}}^{-1} \underline{f}_i \underline{f}_i^T \underline{\underline{M}}_i^{-1} \underline{f}_i .$$

In the middle of the last term of the right hand side, the matrix $W_i \underline{f}_i \underline{f}_i^T$ is equal to $(\underline{\underline{M}} - \underline{\underline{M}}_i)$ according to eq. /A.1.6/. Therefore,

$$\frac{W_i^2}{W_i^* W_i^{**}} = 1 + W_i \underline{f}_i^T \underline{\underline{M}}_i^{-1} \underline{f}_i - W_i \underline{f}_i^T \underline{\underline{M}}^{-1} \underline{f}_i - W_i \underline{f}_i^T \underline{\underline{M}}^{-1} (\underline{\underline{M}} - \underline{\underline{M}}_i) \underline{\underline{M}}_i^{-1} \underline{f}_i =$$

$$= 1 + W_i \underline{f}_i^T (\underline{\underline{M}}_i^{-1} - \underline{\underline{M}}^{-1}) \underline{f}_i - W_i \underline{f}_i^T (\underline{\underline{M}}_i^{-1} - \underline{\underline{M}}^{-1}) \underline{f}_i = 1$$

as stated by eq. /A.1.12/.

In order to prove eq. /A.1.13/ we calculate first

$$Q - W_i (y_i - \tilde{y}_i)^2 = \sum_{j \neq i} W_j (\Delta y_j - \Delta \underline{a}^T \underline{f}_j)^2 = \sum_{j \neq i} W_j \left[(\Delta y_j - \Delta \underline{a}_i^T \underline{f}_j) + (\Delta \underline{a}_i^T - \Delta \underline{a}^T) \underline{f}_j \right]^2 =$$

$$= \sum_{j \neq i} W_j (\Delta y_j - \Delta \underline{a}_i^T \underline{f}_j)^2 + 2 (\Delta \underline{a}_i^T - \Delta \underline{a}^T) \sum_{j \neq i} W_j (\Delta y_j - \Delta \underline{a}_i^T \underline{f}_j) \underline{f}_j +$$

$$+ \sum_{j \neq i} W_j \left[(\Delta \underline{a}_i^T - \Delta \underline{a}^T) \underline{f}_j \right]^2 .$$

According to eq. /A.1.8/, the first term is equal to Q_i. Using eq. /A.1.7/, the last term may be transformed:

$$\sum_{j\neq i} W_j[(\Delta\underline{a}_i^T-\Delta\underline{a}^T)\underline{f}_j][\underline{f}_j^T(\Delta\underline{a}_i-\Delta\underline{a})] = (\Delta\underline{a}_i^T-\Delta\underline{a}^T)\underline{\underline{M}}_i(\Delta\underline{a}_i-\Delta\underline{a}).$$

We show that the second term vanishes. Indeed, it follows from eqs./A.1.6/ and /A.1.7/ that the sum in it may be written as the difference of the following two sums:

$$\sum_{j\neq i} W_j\Delta y_j\underline{f}_j = \underline{\underline{M}}_i\Delta\underline{a}_i$$

and

$$\sum_{j\neq i} W_j(\Delta\underline{a}_i^T\underline{f}_j)\underline{f}_j = \sum_{j\neq i} W_j\underline{f}_j(\underline{f}_j^T\Delta\underline{a}_i) = \sum_{j\neq i} W_j(\underline{f}_j\underline{f}_j^T)\Delta\underline{a}_i = \underline{\underline{M}}_i\Delta\underline{a}_i \ .$$

In this way, we obtained that

$$Q-W_i(y_i-\tilde{y}_i)^2 = Q_i +(\Delta\underline{a}_i^T-\Delta\underline{a}^T)\underline{\underline{M}}_i(\Delta\underline{a}_i-\Delta\underline{a}). \qquad /A.1.17/$$

From eqs. /A.1.6/ and /A.1.7/, we get that

$$\underline{\underline{M}}_i(\Delta\underline{a}_i-\Delta\underline{a}) = \underline{\underline{M}}\Delta\underline{a}-W_i\Delta y_i\underline{f}_i-\underline{\underline{M}}_i\Delta\underline{a} = (\underline{\underline{M}}-\underline{\underline{M}}_i)\Delta\underline{a}-W_i\Delta y_i\underline{f}_i = W_i\underline{f}_i\underline{f}_i^T\Delta\underline{a} - W_i\Delta y_i\underline{f}_i =$$

$$= -W_i(\Delta y_i-\underline{f}_i^T\Delta\underline{a})\underline{f}_i = -W_i(y_i-\tilde{y}_i)\underline{f}_i \ .$$

which, when used in eq. /A.1.17/, leads to the following:

$$Q-W_i(y_i-\tilde{y}_i)^2 = Q_i+(\Delta\underline{a}_i^T-\Delta\underline{a}^T)\underline{\underline{M}}_i\underline{\underline{M}}_i^{-1}\underline{\underline{M}}_i(\Delta\underline{a}_i-\Delta\underline{a}) = Q_i+W_i^2(y_i-\tilde{y}_i)^2\underline{f}_i^T\underline{\underline{M}}_i^{-1}\underline{f}_i \ .$$

Taking into account eqs. /A.1.10/ to /A.1.12/, this may be reduced to eq. /A.1.13/:

$$Q_i = Q - W_i(y_i-\tilde{y}_i)^2(1+W_i\underline{f}_i^T\underline{\underline{M}}_i^{-1}\underline{f}_i) = Q - \frac{W_i^2}{W_i^{**}}(y_i-\tilde{y}_i)^2 = Q-W_i^*(y_i-\tilde{y}_i)^2 =$$

$$= Q - t_i^2\,\frac{Q}{n-m} = Q\left(1 - \frac{t_i^2}{n-m}\right) \ .$$

Finally, we have to calculate the difference on the left hand side of eq. /A.1.14/. Using again eqs. /A.1.6/ and /A.1.7/, this is equal to

$$\Delta y_i-\Delta\underline{a}_i^T\underline{f}_i = \Delta y_i-\Delta\underline{a}^T\underline{\underline{M}}\underline{\underline{M}}_i^{-1}\underline{f}_i + W_i\Delta y_i\underline{f}_i^T\underline{\underline{M}}_i^{-1}\underline{f}_i =$$

$$= \Delta y_i - \Delta \underline{a}^T (\underline{\underline{M}}_i + W_i \underline{f}_i \underline{f}_i^T) \underline{\underline{M}}_i^{-1} \underline{f}_i + W_i \Delta y_i \underline{f}_i^T \underline{\underline{M}}_i^{-1} \underline{f}_i =$$

$$= (\Delta y_i - \Delta \underline{a}^T \underline{f}_i)(1 + W_i \underline{f}_i^T \underline{\underline{M}}_i^{-1} f_i) = (y_i - \tilde{y}_i)(1 + W_i \underline{f}_i^T \underline{\underline{M}}_i^{-1} \underline{f}_i) \ .$$

If eqs. /A.1.10/ to A.1.12/ are also taken into account, we get that

$$(\Delta y_i - \Delta \underline{a}_i^T \underline{f}_i) \sqrt{W_i^{**}} = (y_i - \tilde{y}_i) \sqrt{W_i^{**}} \frac{W_i}{W_i^{**}} = (y_i - \tilde{y}_i) \sqrt{W_i^*} = t_i \sqrt{\frac{Q}{n-m}} \ ,$$

as stated by eq. /A.1.14/.

These derivations show that eqs. /A.1.12/ to /A.1.14/ could be proved by pure algebra. Consequently, the validity of eq. /III.2.9/ depends only on the approximations made before, namely in eq. /A.1.3a/. Therefore, the only limitation is that we neglected the bias and we calculate the elements of matrix $\underline{\underline{F}}$ at $\hat{\underline{a}}$ instead of at $\underline{a}$. This is however an order of approximation which in considered to be allowed for throughout the present paper. As a matter of fact, formula /III.2.9/ is found to hold to an excellent approximation in practice.

APPENDIX 2.

THE QUANTILES OF THE φ-DISTRIBUTION*

The φ-ratio was introduced by eq. /IV.2.19/. Its distribution is not generally known, therefore, we give here the algorithm of computing its quantiles. For simplicity, we write ℓ for (n_k-m) and k for (L-k). By definition

$$\varphi_{\ell,k} = \frac{\chi_k/\sqrt{k}}{\chi^2_\ell/\ell} \quad , \qquad k \leq \ell \qquad /A.2.1/$$

Define the function

$$F_{k\ell}(z) = P\{\frac{\chi_k}{\chi^2_\ell} < z\} \ . \qquad /A.2.2/$$

Now, the quantile γ_φ is to be found as the solution of the equation

$$F_{k\ell}(\frac{\sqrt{k}}{\ell}\,\gamma_\varphi) = 1-\varepsilon \ . \qquad /A.2.3/$$

In an elementary way, it may be derived that

$$f_{k\ell}(z) = \frac{dF_{k\ell}(z)}{dz} = \frac{z^{k-1}}{2^{\frac{\ell+k}{2}-1}\,\Gamma(\frac{\ell}{2})\,\Gamma(\frac{k}{2})} \int_0^\infty x^{k+\frac{\ell}{2}-1}\, e^{-\frac{1}{2}(x+x^2z^2)}\, dx \ . \qquad /A.2.4/$$

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* The algorithm and the subroutine for the calculation of these quantiles were elaborated by G.Németh.

These function satisfy the following recurrence relations:

$$F_{k\ell}(z) = F_{k,\ell-2}(z) + \frac{2z}{\ell-2} f_{k,\ell-2}(z) \qquad /A.2.5/$$

and

$$(\ell-2)(\ell-4)z^2 f_{k\ell}(z) = (k+\tfrac{\ell}{2}-2)f_{k,\ell-4}(z) - (\tfrac{\ell}{2}-2)f_{k,\ell-2}(z). \qquad /A.2.6/$$

These formulae could be used to reach any (k,ℓ) starting from some of $k,\ell=1,2,3,4$. This is, however, impractical because the starting functions are not analytical. Therefore, the following procedure was used.

It may be shown on the basis of eq. /A.2.6/ that the ratios

$$V_m = \frac{f_{k,\ell+2m+2}(z)}{f_{k,\ell+2m}(z)} \qquad /A.2.7/$$

satisfy the recurrence relation

$$(\tfrac{\ell}{2} + m)V_m = \frac{k + \ell/2 + m}{1 + 4z^2(\tfrac{\ell}{2} + m+1)\, V_{m+1}} . \qquad /A.2.8/$$

For a large m, this goes over asymptotically in

$$V_m \approx \frac{\sqrt{\ell/2 + k-1 + m}}{2z(\tfrac{\ell}{2} + m)} . \qquad /A.2.9/$$

Starting from there, all v_m can be computed for m=0,1,2,... Then we have that

$$f_{k,\ell+2m}(z) = f_{k\ell}(z) \prod_{i=0}^{m-1} V_i \qquad /A.2.10/$$

$f_{k,\ell}(z)$ itself is computed from the following normalization formula:

$$\sum_{m=0}^{\infty} f_{k,\ell+4m}(z) \frac{\Gamma(\frac{\ell}{2}+2m)}{\Gamma(\frac{\ell}{2})m\,!} (2z^2)^m \equiv \frac{z^{k-1}\, 2^{\frac{k}{2}+1}\, \Gamma(k+\frac{\ell}{2})}{\Gamma(\frac{\ell}{2})\, \Gamma(\frac{k}{2})} . \qquad /A.2.11/$$

The proof of this identity is straightforward if $f_{k,\ell+4m}(z)$ is substituted from eq. /A.2.4/. Finally, $F_{k\ell}(z)$ is obtained as

$$F_{k\ell}(z) = 1 - 2z \sum_{m=0}^{\infty} \frac{f_{k,\ell+2m}(z)}{\ell+2m} . \qquad /A.2.12/$$

It may be directly verified that this satisfies the recurrence relation /A.2.5/.

Eq. /A.2.3/ is solved by iteration. Numerical difficulties arise when the ratio ℓ/k is large. In this case, the asymptotics given by /A.2.9/ is reached only for very large m.

Table A.2. gives the quantile γ_φ for characteristic values of k, ℓ and ε.

APPENDIX 3.

PROOF OF EQ. (IV.1.18)

We have by definition that

$$\Gamma_{min} = \sum_{\ell=1}^{L} \sum_{\ell'=1}^{L} \omega_{\ell\ell'}(p_\ell - \tilde{p}_o)(p_{\ell'} - \tilde{p}_o) \qquad /A.3.1/$$

where $\tilde{p}_o$ is given by eq. /IV.1.15/. This expression may be rewritten by putting $(p_\ell - p_o)$ and $(\tilde{p}_o - p_o)$ for p_ℓ and $\tilde{p}_o$, respectively. Therefore, nothing changes if we, for simplicity, denote these differences by p_ℓ and $\tilde{p}_o$ /for the derivations of the present appendix only/. After this change of notations, we may say that p_ℓ and $\tilde{p}_o$ have zero means.

Matrix $\underline{\underline{C}}^{-1}$ may be diagonalized as

$$\underline{\underline{C}}^{-1} = \underline{\underline{U}}^{-1} \, \underline{\underline{\Lambda}} \, \underline{\underline{U}} \qquad /A.3.2/$$

where the diagonal matrix $\underline{\underline{\Lambda}}$ is built up from the reciprocals of the eigenvalues λ_ℓ of matrix $\underline{\underline{C}}$ and $\underline{\underline{U}}$ is and orthogonal matrix i.e. $\underline{\underline{U}}^T = \underline{\underline{U}}^{-1}$. Matrix $\underline{\underline{C}}$ is positive definite. Therefore, all its eigenvalues are positive, so that it is legitime to form the diagonal matrix $\underline{\underline{\Lambda}}^{1/2}$ from $1/\sqrt{\lambda_\ell}$ as elements. Furthermore, we define vector $\underline{e}$ the elements of which are all equal to 1 and vector $\underline{p}$ the elements of which are p_ℓ. In these notations,

$$\Gamma_{min} = (\underline{p}^T - \tilde{p}_o \underline{e}^T) \, \underline{\underline{C}}^{-1} (\underline{p} - \tilde{p}_o \underline{e}) \qquad /A.3.3/$$

and eq. /IV.1.15/ may be written as

$$\tilde{p}_o = \frac{\underline{p}^T \, \underline{\underline{C}}^{-1} \, \underline{e}}{\underline{e}^T \, \underline{\underline{C}} \, \underline{e}} . \qquad /A.3.4/$$

After some elementary calculation, eq. /A.3.3/ goes over in

$$\Gamma_{min} = \underline{p}^T \underline{\underline{C}}^{-1} \underline{p} - \frac{(\underline{p}^T \underline{\underline{C}}^{-1} \underline{e})^2}{\underline{e}^T \underline{\underline{C}}^{-1} \underline{e}} . \qquad /A.3.5/$$

We define now the vectors

$$\underline{q} = \underline{\underline{\Lambda}}^{1/2} \underline{\underline{U}} \underline{p} \qquad /A.3.6/$$

and

$$\underline{r} = \underline{\underline{\Lambda}}^{1/2} \underline{\underline{U}} \underline{e} . \qquad /A.3.7/$$

Using these expressions in eq. /A.3.5/, we obtain

$$\Gamma_{min} = \underline{q}^T \underline{q} - \frac{(\underline{q}^T \underline{r})^2}{\underline{r}^T \underline{r}} = \sum_{\ell=1}^{L} q_\ell^2 - \frac{(\sum_{\ell=1}^{L} q_\ell r_\ell)^2}{\sum_{\ell=1}^{L} r_\ell^2} . \qquad /A.3.8/$$

There exists now an orthogonal matrix $\underline{\underline{A}}$ the first row of which is given by

$$\{\underline{\underline{A}}\}_{1\ell} = \frac{r_\ell}{\sqrt{\underline{r}^T \underline{r}}} . \qquad /A.3.9/$$

If this matrix is applied to vector $\underline{q}$, the resulting vector

$$\underline{z} = \underline{\underline{A}} \underline{q} \qquad /A.3.10/$$

will have as the first element

$$z_1 = \frac{\underline{q}^T \underline{r}}{\sqrt{\underline{r}^T \underline{r}}} \qquad /A.3.11/$$

and, using eq. /A.3.10/, we have that

$$\underline{q}^T \underline{q} = (\underline{\underline{A}}^{-1} \underline{z})^T (\underline{\underline{A}}^{-1} \underline{z}) = \underline{z}^T \underline{z} = \sum_{\ell=1}^{L} z_\ell^2 \qquad /A.3.12/$$

where it was taken into account that $\underline{\underline{A}}$ is orthogonal i.e. $\underline{\underline{A}}^T = \underline{\underline{A}}^{-1}$. Putting $\underline{q}^T \underline{q}$ from eq. /A.3.12/ and z_1 from eq. /A.3.10/ in eq. /A.3.8/, we obtain

$$\Gamma_{min} = \sum_{\ell=1}^{L} z_\ell^2 - z_1^2 = \sum_{\ell=2}^{L} z_\ell^2 . \qquad /A.3.13/$$

If we can now show that the z_ℓ are N(0,1) and they are independent from each other, eq. /IV.1.18/ is proved because the number of terms is (L-1) on the right hand side of eq. /A.3.13/. We remind that p_ℓ stands for Δp_ℓ in this appendix so that eq. /IV.1.9/ may be rewritten as

$$\langle \underline{p}\underline{p}^T \rangle = \underline{\underline{C}} = \underline{\underline{U}}^{-1} \underline{\underline{\Lambda}}^{-1} \underline{\underline{U}} \qquad /A.3.14/$$

and

$$\langle \underline{p} \rangle = 0. \qquad /A.3.15/$$

From eqs. /A.3.6/ and /A.3.10/, $\underline{z}$ may be expressed in the form

$$\underline{z} = \underline{\underline{A}}\, \underline{\underline{\Lambda}}^{1/2}\, \underline{\underline{U}}\, \underline{p} \; . \qquad /A.3.16/$$

The mean of $\underline{z}$ is zero trivially /see eq. /A.3.15//. Using eq. /A.3.14/, we have for the covariance matrix

$$\langle \underline{z}\underline{z}^T \rangle = \underline{\underline{A}}\, \underline{\underline{\Lambda}}^{1/2}\, \underline{\underline{U}}\, \langle \underline{p}\underline{p}^T \rangle \underline{\underline{U}}^{-1}\, \underline{\underline{\Lambda}}^{1/2}\, \underline{\underline{A}}^{-1} = \underline{\underline{A}}\, \underline{\underline{\Lambda}}^{1/2}\, \underline{\underline{U}}\, \underline{\underline{U}}^{-1}\, \underline{\underline{\Lambda}}^{-1} \underline{\underline{U}}\underline{\underline{U}}^{-1}\, \underline{\underline{\Lambda}}^{1/2}\, \underline{\underline{A}}^{-1} = \underline{\underline{E}} \; .$$

Consequently, the covariance matrix of $\underline{z}$ is the unit matrix. This means that its elements are independent from each other and their variances are equal to 1.

APPENDIX 4.

EFFICIENCY OF THE ESTIMATE $\tilde{p}_o = p_1$

It was stated in section I.1 that the maximum likelihood estimates are asymptotically efficient. For the point drop technique, this means that the estimate $\tilde{p}_o = p_1$ as given by eq. /IV.1.23a/ has the minimum variance in the limit when L goes to infinity. This statement would apply to our case only if the p_ℓ were independent from each other. Actually, this is far from being true. It is therefore not without interest to raise the question whether some better estimate could be found. In this Appendix, we shall study estimates of the form

$$\tilde{p} = \sum_{\ell=1}^{L} s_\ell p_\ell \qquad /A.4.1/$$

with

$$\sum_{\ell=1}^{L} s_\ell = 1 \qquad /A.4.2/$$

i.e. we ask whether some suitably chosen weighted averages might be better than eq. /IV.1.23a/. It is trivial that, for any set of the weights s_ℓ, the estimate is unbiased:

$$\langle \tilde{p} \rangle = \sum_{\ell=1}^{L} s_\ell \langle p_\ell \rangle = p_o \sum_{\ell=1}^{L} s_\ell = p_o \ . \qquad /A.4.3/$$

Any non-linear function of the p_ℓ has the property of being biased. It can be unbiased only in singular cases. Hence, the form /A.4.1/ represents sufficiently generally the class of unbiased estimates. As a matter of fact, it is hard to dream up any reasonable unbiased estimate which would have a form other than the weighted average.

The variance of $\tilde{p}$ may be calculated taking into account eq. /IV.1.7b/:

$$\langle (\Delta\tilde{p})^2 \rangle = \sum_{\ell=1}^{L} s_\ell^2 (\Delta p_\ell)^2 + 2 \sum_{\ell=1}^{L-1} s_\ell (\Delta p_\ell)^2 \sum_{\ell'=\ell+1}^{L} s_{\ell'} \ . \qquad /A.4.4/$$

Eq. /IV.1.23a/ corresponds to the following weighting:

$$s_1 = 1, \quad s_2 = s_3 = \ldots = s_L = 0. \qquad /A.4.5/$$

In this case, of course, the variance is

$$\langle(\Delta\tilde{p})^2\rangle = (\Delta p_1)^2 .$$

We show now that $\langle(\Delta\tilde{p})^2\rangle$ is always larger than $(\Delta p_1)^2$ if the weighting is different from the set given by eq. /A.4.5/.

From formula /IV.1.8/, we have that

$$\Delta p_\ell \leq \Delta p_{\ell+1} . \qquad /A.4.6/$$

Therefore,

$$\langle(\Delta\tilde{p})^2\rangle \geq (\Delta p_1)^2 \sum_{\ell=1}^{L} s_\ell^2 + 2(\Delta p_1)^2 \sum_{\ell=1}^{L-1} s_\ell \sum_{\ell'=\ell+1}^{L} s_{\ell'} =$$

$$= (\Delta p_1)^2 \Big(\sum_{\ell=1}^{L} s_\ell\Big)^2 = (\Delta p_1)^2, \qquad /A.4.7/$$

consequently, $\langle(\Delta\tilde{p})^2\rangle$ is really bounded by $(\Delta p_1)^2$.

We have left to prove that this lower bound is reached only for the weights given by eq. /A.4.5/. Combining formulae /A.4.4/ /A.4.7/, we get that

$$\langle(\Delta\tilde{p})^2\rangle - (\Delta p_1)^2 = \sum_{\ell=2}^{L} s_\ell^2[(\Delta p_\ell)^2-(\Delta p_1)^2] + 2\sum_{\ell=2}^{L-1} s_\ell[(\Delta p_\ell)^2-(\Delta p_1)^2]\sum_{\ell'=\ell+1}^{L} s_{\ell'},$$

/A.4.8/

Using again the unequality /A.4.6/, we may write that /cf. /A.4.7//

$$\langle(\Delta\tilde{p})^2\rangle - (\Delta p_1)^2 \geq [(\Delta p_2)^2 - (\Delta p_1)^2]\Big(\sum_{\ell=2}^{L} s_\ell\Big)^2 = [(\Delta p_2)^2 - (\Delta p_1)^2](1-s_1)^2 \geq 0$$

/A.4.9/

It follows from this that $\langle(\Delta\tilde{p})^2\rangle$ may be equal to $(\Delta p_1)^2$ only in two cases:

- when $\Delta p_2 = \Delta p_1$,
- or when $s_1 = 1$: this is just eq. /A.4.5/.

We have found that, unless the degenerated case occurs, the variance reaches its lower bound only for the weighting defined by eq. /A.4.5/. This kind of degeneration may be left out of consideration. This would mean that the point/s/ dropped in step 2 contain no information because the correlation coefficient of p_1 and p_2 is equal to 1 saying that p_1 and p_2 are identical. Therefore, step 2 is to be left out. Consequently, only the case $s_1=1$ is of interest. With that, we proved the efficiency of the maximum likelihood estimate /IV.1.23a/.

Of course, we could have gone the other way round: we could have searched the minimum of $<(\Delta\tilde{p})^2>$ taking into account the auxiliary condition /A.4.2/. It is straightforward to show that the minimum is really reached by /A.4.5/.

APPENDIX 5.

COMPUTATION OF Γ_k

Eq. /IV.1.26/ defines Γ_k in terms of the elements of the inverse of matrix $\underline{\underline{C}}^k$. As this computation has to be carried out for k=1,2,...,L-1, it is desirable to have an algorithm not necessitating the time consuming matrix inversions. Such an algorithm is the following.

The quantities

$$z_\ell = \sum_{\ell'=k}^{L} \omega_{\ell\ell'}(p_{\ell'}-p_k) \qquad /A.5.1/$$

are calculated first. When they are known, Γ_k may be obtained by

$$\Gamma_k = \sum_{\ell=k}^{L} z_\ell (p_\ell - p_k) \ . \qquad /A.5.2/$$

Since $\omega_{\ell\ell'}$ is an element of matrix $(\underline{\underline{C}}^k)^{-1}$, the numbers z_ℓ are the solutions of the following set of equations:

$$\sum_{\ell'=k}^{L} \{\underline{\underline{C}}^k\}_{\ell\ell'} z_{\ell'} = p_\ell - p_k \ . \qquad /A.5.3/$$

$$\ell = k, k+1, \ldots, L$$

Putting in here the elements of $\underline{\underline{C}}^k$ from eq. /IV.1.22a/, this goes over in

equation for $\ell = k$:

$$\sum_{\ell'=k}^{L} z_{\ell'} = 0 \qquad /A.5.4a/$$

equation for $\ell > k$:

$$\sum_{\ell'=k}^{\ell-1} (\Delta p_{\ell'})^2 z_{\ell'} + (\Delta p_\ell)^2 \sum_{\ell'=\ell}^{L} z_{\ell'} = p_\ell - p_k \ . \qquad /A.5.4b/$$

In order to solve this set of equations. we introduce the notation

$$\mu_\ell = \sum_{\ell'=\ell}^{L} z_{\ell'} \quad . \qquad /A.5.5/$$

z_ℓ may be expressed in terms of μ_ℓ as

$$z_\ell = \begin{cases} \mu_\ell - \mu_{\ell+1} & \text{if} \quad \ell \leq L-1 \\ \mu_L & \text{if} \quad \ell = L \end{cases} \qquad /A.5.6/$$

It follows from eq. /A.5.4a/ that

$$\mu_k = 0 \qquad /A.5.7/$$

If we apply eq. /A.5.4b/ for $\ell=k+1$, we get

$$(\Delta p_k)^2 \, z_k + (\Delta p_{k+1})^2 \, \mu_{k+1} = p_{k+1} - p_k \, .$$

From eqs. /A.5.6/ and /A.5.7/, we have that $z_k = -\mu_{k+1}$, so that this last equation goes over in

$$\mu_{k+1} = \frac{p_{k+1} - p_k}{(\Delta p_{k+1})^2 - (\Delta p_k)^2} \, . \qquad /A.5.8/$$

Now, write down eq. /A.5.4b/ for $(\ell+1)$ instead of ℓ, and substract eq. /A.5.4b/ from it ($\ell \leq L-1$). This yields

$$(\Delta p_\ell)^2 \, z_\ell + (\Delta p_{\ell+1})^2 \mu_{\ell+1} - (\Delta p_\ell)^2 \, \mu_\ell = p_{\ell+1} - p_\ell \, .$$

If it is combined with eq. /A.5.6/, we obtain

$$\mu_{\ell+1} = \frac{p_{\ell+1} - p_\ell}{(\Delta p_{\ell+1})^2 - (\Delta p_\ell)^2} \qquad /A.5.9/$$

$$\ell = k, k+1, \ldots, L-1$$

Eq. /A.5.4b/ holds only for $\ell \geq k+1$, so this last result would also be valid only for $\ell \geq k+1$ but it is in fact the same as eq. /A.5.8/ for $\ell=k$. Therefore, eq. /A.5.9/ gives $\mu_{\ell+1}$ for all relevant ℓ .

We come now to the calculation of Γ_k. In view of eqs. /A.5.4a/ and /A.5.6/, eq. /A.5.2/ may be rewritten as

$$\Gamma_k = \sum_{\ell=k}^{L} z_\ell(p_\ell - p_k) = \sum_{\ell=k}^{L} z_\ell p_\ell = p_L\mu_L + \sum_{\ell=k}^{L-1} (\mu_\ell - \mu_{\ell+1})p_\ell \ .$$

If the identity

$$(\mu_\ell - \mu_{\ell+1})p_\ell = \mu_\ell p_\ell - \mu_{\ell+1} p_{\ell+1} + \mu_{\ell+1}(p_{\ell+1} - p_\ell)$$

is taken into account, the expression for Γ_k goes over in

$$\Gamma_k = p_L\mu_L + \sum_{\ell=k}^{L-1} \mu_\ell p_\ell - \sum_{\ell=k}^{L-1} \mu_{\ell+1}p_{\ell+1} + \sum_{\ell=k}^{L-1} \mu_{\ell+1}(p_{\ell+1} - p_\ell) = \mu_k p_k + \sum_{\ell=k}^{L-1} \mu_{\ell+1}(p_{\ell+1} - p_\ell).$$

$\mu_k = 0$ according to eq. /A.5.7/ and $\mu_{\ell+1}$ is given by eq. /A.5.9/ so that

$$\Gamma_k = \sum_{\ell=k}^{L-1} \frac{(p_{\ell+1} - p_\ell)^2}{(\Delta p_{\ell+1})^2 - (\Delta p_\ell)^2} \qquad /A.5.10/$$

This is a very convenient formula.

We note yet that eq. /IV.1.27/ simply follows from that. In fact, it may be shown on the basis of eq. /IV.1.22a/ that

$$\xi_\ell = \frac{p_{\ell+1} - p_\ell}{\sqrt{(\Delta p_{\ell+1})^2 - (\Delta p_\ell)^2}} \qquad /A.5.11/$$

is $N(0,1)$ and ξ_ℓ and $\xi_{\ell'}$ are independent when $\ell \neq \ell'$. Consequently,

$$\Gamma_k = \sum_{\ell=k}^{L-1} \xi_\ell^2 = \chi^2_{L-k} \qquad /A.5.12/$$

APPENDIX 6.

THE COVARIANCE OF Q_ℓ AND $Q_{\ell'}$.

Let us denote the i^{th} row of matrix $\underline{\underline{F}}$ by $\underline{f}_i^T$ as in Appendix 1. Then, by analogy with eq. /A.1.2/, we have that

$$Q_\ell = \sum_{i \in I_\ell} w_i (\Delta y_i - \Delta \underline{a}_\ell^T \underline{f}_i)^2 \qquad /A.6.1/$$

and

$$\Delta \underline{a}_\ell = \underline{\underline{M}}_\ell^{-1} \underline{\underline{F}}_\ell^T \underline{\underline{W}}_\ell \Delta \underline{y}_\ell \qquad /A.6.2/$$

/see eq. /II.1.12//. Without restricting the generality, it is sufficient to consider only the unweighted case i.e. when $\underline{\underline{W}} = \underline{\underline{E}}$. In fact, making the following transformations

$$\underline{\underline{W}}^{1/2} \underline{\underline{F}}_\ell = \underline{\underline{F}}'_\ell \qquad \text{and} \qquad \underline{\underline{W}}_\ell^{1/2} \Delta \underline{y}_\ell = \underline{y}'_\ell \qquad /A.6.3/$$

we have that

$$\underline{\underline{M}}_\ell = \underline{\underline{F}}_\ell^T \underline{\underline{W}}_\ell \underline{\underline{F}}_\ell = \underline{\underline{F}}_\ell'^T \underline{\underline{F}}'_\ell \qquad /A.6.4a/$$

$$\Delta \underline{a}_\ell = \underline{\underline{M}}_\ell^{-1} \underline{\underline{F}}_\ell'^T \underline{y}'_\ell \qquad /A.6.4b/$$

and

$$Q_\ell = \sum_{i \in I_\ell} (y'_i - \Delta \underline{a}_\ell^T \underline{f}'_i)^2 \ . \qquad /A.6.4c/$$

These formulae correspond exactly to the unweighted case. For simplicity, the primes will be omitted in the following.

The y_i are $N(0,\sigma)$ characterized by

$$\langle y_i \rangle = \langle y_i^3 \rangle = 0 \ , \qquad \langle y_i^2 \rangle = \sigma^2 \ , \qquad \langle y_i^4 \rangle = 3\sigma^4 , \qquad /A.6.5/$$

/Do not forget that we have written here already y_i for $y'_i = \sqrt{w_i}\ \Delta y_i$!/

If the squares in eq. /A.6.4c/ are explicitely calculated and eqs. /A.6.4a/ and /A.6.4b/ are taken into account, one gets

$$Q_\ell = \underline{Y}_\ell^T \underline{\underline{P}}_\ell \underline{Y}_\ell = \sum_{i\in I_\ell} \sum_{j\in I_\ell} P_{ij}^\ell \, y_i y_j \qquad /A.6.6/$$

where

$$\underline{\underline{P}}_\ell = \underline{\underline{E}}_\ell - \underline{\underline{F}}_\ell \, (\underline{\underline{F}}_\ell^T \underline{\underline{F}}_\ell)^{-1} \underline{\underline{F}}_\ell^T \, . \qquad /A.6.7/$$

Now, write down eq. /A.6.6/ for $\ell=\ell'$ and then form the product $Q_\ell Q_{\ell'}$, as

$$Q_\ell Q_{\ell'} = \sum_{i\in I_\ell} \sum_{j\in I_\ell} \sum_{i'\in I_{\ell'}} \sum_{j'\in I_{\ell'}} P_{ij}^\ell \, P_{i'j'}^{\ell'} \, y_i \, y_j \, y_{i'} \, y_{j'} \qquad /A.6.8/$$

Since y_i and y_j are independent when $i\neq j$ and odd powers of y_i have zero expectation according to eq. /A.6.5/, most of the terms on the right hand side of eq. /A.6.8/ will have zero expectation. The exceptions are the following three types of combinations:

1/ $i=j$ and $i'=j'$
2/ $i=i'$ and $j=j'$
3/ $i=j'$ and $j=i'$

The symmetry of matrices $\underline{\underline{P}}$ assures that the sum of terms of types 2/ and 3/ are equal. In order to collect the terms of all these three types, we devide the summation for i and j in four parts taking into account that I_ℓ, c I_ℓ /see figure A.1/

$$Q_\ell Q_{\ell'} = a + b + c + d \qquad /A.6.9/$$

where

a: $\sum_{i\in I_\ell}$, $\sum_{j\in I_\ell}$,

b: $\sum_{i\in I_\ell}$, $\sum_{j\in I_\ell - I_{\ell'}}$,

c: $\sum_{i\in I_\ell - I_{\ell'}}$, $\sum_{j\in I_\ell}$,

d: $\sum_{i\in I_\ell - I_{\ell'}}$, $\sum_{j\in I_\ell - I_{\ell'}}$,

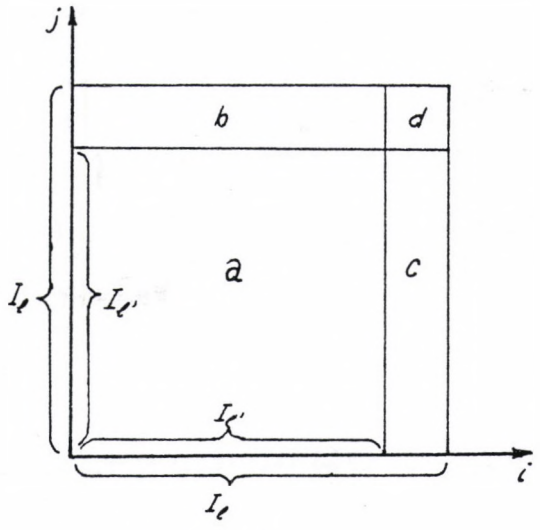


Fig. A.1.

In part b, j is different from all the subscripts i, i' and j' so that its expectation vanishes. In part c, the analogous thing happens to i, consequently the expectation of part c vanishes as well. In part a, all three types are possible, therefore

$$\langle a\rangle = \sum_{i\in I_\ell,} \sum_{j\in I_\ell,} P^{\ell}_{ii} P^{\ell'}_{jj} \langle y_i^2 y_j^2\rangle + 2 \sum_{\substack{i\in I_\ell, \\ i\neq j}} \sum_{j\in I_\ell,} P^{\ell}_{ij} P^{\ell'}_{ij} \langle y_i^2 y_j^2\rangle . \qquad /A.6.10/$$

Here, the first sum corresponds to type 1/, while the second one to types 2/ and 3/. Finally, only type 1/ is possible in part d, therefore,

$$\langle d\rangle = \sum_{i\in I_\ell - I_\ell,} \sum_{j\in I_\ell,} P^{\ell}_{ii} P^{\ell'}_{jj} \langle y_i^2 y_j^2\rangle . \qquad /A.6.11/$$

With that and with eq. /A.6.9/, we are now able to calculate the expectation of $Q_\ell Q_{\ell'}$:

$$\langle Q_\ell Q_{\ell'}\rangle = \langle a\rangle + \langle d\rangle = \sum_{i\in I_\ell} \sum_{j\in I_{\ell'},} P^{\ell}_{ii} P^{\ell'}_{jj} \langle y_i^2 y_j^2\rangle + 2 \sum_{\substack{i\in I_\ell, \\ i\neq j}} \sum_{j\in I_{\ell'},} P^{\ell}_{ij} P^{\ell'}_{ij} \langle y_i^2 y_j^2\rangle . \qquad /A.6.12/$$

On the basis of formula /A.6.5/, $\langle y_i^2 y_j^2\rangle$ may be written as

$$\langle y_i^2 y_j^2\rangle = \sigma^4 + 2\sigma^4 \delta_{ij} . \qquad /A.6.13/$$

Putting this in eq. /A.6.12/, we get

$$\frac{1}{\sigma^4} \langle Q_\ell Q_{\ell'}\rangle = \sum_{i\in I_\ell} \sum_{j\in I_{\ell'},} P^{\ell}_{ii} P^{\ell'}_{jj} + 2 \sum_{i\in I_\ell,} P^{\ell}_{ii} P^{\ell'}_{ii} +$$

$$+ 2 \sum_{\substack{i\in I_\ell, \\ i\neq j}} \sum_{j\in I_{\ell'},} P^{\ell}_{ij} P^{\ell'}_{ij} = \sum_{i\in I_\ell} \sum_{j\in I_{\ell'},} P^{\ell}_{ii} P^{\ell'}_{jj} + 2 \sum_{i\in I_\ell,} \sum_{j\in I_{\ell'},} P^{\ell}_{ij} P^{\ell'}_{ij}$$

/A.6.14/

Taking the expectations of both sides of eq. /A.6.6/, we obtain that

$$\langle Q_\ell\rangle = \sigma^2 \sum_{i\in I_\ell} P^{\ell}_{ii} . \qquad /A.6.15/$$

Using these last two formulae, the covariance of Q_ℓ and $Q_{\ell'}$, is given by

$$\frac{1}{\sigma^4}\langle q_\ell q_{\ell'}\rangle = \frac{1}{\sigma^4}(\langle Q_\ell Q_{\ell'}\rangle - \langle Q_\ell\rangle\langle Q_{\ell'}\rangle) = 2 \sum_{i\in I_\ell,} \sum_{j\in I_{\ell'},} P^{\ell}_{ij} P^{\ell'}_{ij} \cdot \qquad /A.6.16/$$

Formally, we have solved our problem: we have an explicite expression for the covariance. This formal expression may be, however, simplified. For that purpose, we write eq. /A.6.7/ by elements:

$$P^{\ell}_{ij} = \delta_{ij} - \sum_{k_1} \sum_{k_2} f_{ik_1} f_{jk_2} \omega^{\ell}_{k_1k_2} \qquad /A.6.17/$$

where $\omega^{\ell}_{k_1k_2}$ is an element of matrix $(\underline{\underline{F}}^T_\ell \underline{\underline{F}}_\ell)^{-1}$:

$$\omega^{\ell}_{k_1k_2} = \{(\underline{\underline{F}}^T_\ell \underline{\underline{F}}_\ell)^{-1}\}_{k_1k_2} \qquad /A.6.18/$$

and subscripts k_1 and k_2 go through values 1 to m. Later on, we shall need the matrix elements

$$\mu^{\ell}_{k_1k_2} = \{\underline{\underline{F}}^T_\ell \underline{\underline{F}}_\ell\}_{k_1k_2} = \sum_{i\in I_\ell} f_{ik_1} f_{ik_2} \cdot \qquad /A.6.19/$$

Since these latter quantities are elements of matrices which are inverses to each other, it holds that

$$\sum_k \omega^{\ell}_{k_1k} \mu^{\ell}_{kk_2} = \delta_{k_1k_2} \cdot \qquad /A.6.20/$$

Using eq. /A.6.17/ for ℓ and ℓ' , we have that

$$\sum_{i\in I_\ell,} \sum_{j\in I_{\ell'},} P^{\ell}_{ij} P^{\ell'}_{ij} = n_{\ell'} - \sum_{k_1} \sum_{k_2} \Big(\sum_{i\in I_{\ell'},} f_{ik_1} f_{ik_2} \omega^{\ell}_{k_1k_2} +$$

$$+ \sum_{i\in I_{\ell'},} f_{ik_1} f_{ik_2} \omega^{\ell'}_{k_1k_2}\Big) +$$

$$+ \sum_{i\in I_\ell,} \sum_{j\in I_{\ell'},} \sum_{k_1} \sum_{k_2} \sum_{k_1'} \sum_{k_2'} f_{ik_1} f_{jk_2} f_{ik_1'} f_{jk_2'} \omega^{\ell}_{k_1k_2} \omega^{\ell'}_{k_1'k_2'}$$

/A.6.21/

In each sum here, summation over i results in some element $\mu^{\ell'}_{kk}$, while summation over j results in $\mu^{\ell'}_{k_2k_2'}$. In view of eq. /A.6.20/, summation over k_1 and k_2 of the second term of the second sum gives m.

Therefore,

$$\sum_{i\in I_\ell,} \sum_{j\in I_\ell,} p^{\ell}_{ij}\, p^{\ell'}_{ij} = n_{\ell},-m-\sum_{k_1}\sum_{k_2} \mu^{\ell'}_{k_1k_2}\, \omega^{\ell}_{k_1k_2} +$$

$$+ \sum_{k_1}\sum_{k_2}\sum_{k_1'}\sum_{k_2'} \mu^{\ell'}_{k_1k_1'}\, \mu^{\ell'}_{k_2k_2'}\, \omega^{\ell}_{k_1k_2}\, \omega^{\ell'}_{k_1'k_2'} \cdot \qquad /A.6.22/$$

In the last sum, the summation over k_1' is carried out first. According to eq. /A.6.20/, this results in

$$\sum_{k_1'} \mu^{\ell'}_{k_1k_1'}\, \omega^{\ell'}_{k_1'k_2'} = \delta_{k_1k_2'} \cdot$$

Taking this into account, summation over k_2' reduces the last sum to

$$\sum_{k_1}\sum_{k_2}\sum_{k_2'} \mu^{\ell'}_{k_2k_2'}\, \omega^{\ell}_{k_2k_2'}\, \delta_{k_1k_2'} = \sum_{k_1}\sum_{k_2} \mu^{\ell'}_{k_2k_1}\, \omega^{\ell}_{k_1k_2}$$

which is the same as the second sum in eq. /A.6.22/ because matrix $\underline{\underline{F}}^{T}_{\ell},\underline{\underline{F}}_{\ell},$ is symmetric so that $\mu^{\ell'}_{k_2k_1}=\mu^{\ell'}_{k_1k_2}$. Thus, we have shown that

$$\sum_{i\in I_\ell,} \sum_{j\in I_\ell,} p^{\ell}_{ij}\, p^{\ell'}_{ij} = n_{\ell}, - m. \qquad /A.6.23/$$

Putting this in eq. /A.6.16/, we obtain that

$$\langle q_\ell q_{\ell},\rangle = 2\sigma^4(n_{\ell}, - m) \quad \text{if} \quad I_\ell, CI_\ell \qquad /A.6.24/$$

APPENDIX 7.

COMPUTATION AND PROPERTIES OF T_k

The proof of eq. /IV.2.18/ goes essentially along the lines of Appendix 3. We form vector $\underline{q}$ first with components $q_1, q_2, \ldots, q_L$. Matrix $\underline{\underline{S}}$ is diagonalized by the orthogonal matrix $\underline{\underline{U}}$ as

$$\underline{\underline{S}} = \underline{\underline{U}}^{-1} \underline{\underline{\Lambda}} \underline{\underline{U}} \ . \qquad /A.7.1/$$

Vector $\underline{q}$ is transformed to vector $\underline{r}$:

$$\underline{r} = \frac{1}{\sigma^2\sqrt{2}} \underline{\underline{\Lambda}}^{1/2} \underline{\underline{U}} \underline{q} \qquad /A.7.2/$$

or

$$\underline{q} = \sigma^2\sqrt{2}\, \underline{\underline{U}}^T \underline{\underline{\Lambda}}^{-\frac{1}{2}} \underline{r} \ . \qquad /A.7.3/$$

Now, it may be simply shown that

$$\sum_{\ell=1}^{L} \sum_{\ell'=1}^{L} S_{\ell\ell'} q_\ell q_{\ell'} = 2\sigma^4 \sum_{\ell=1}^{L} r_\ell^2 \ . \qquad /A.7.4/$$

Using eq. /IV.2.7/, we put

$$\langle \underline{r}\underline{r}^T \rangle = \frac{1}{2\sigma^4} \underline{\underline{\Lambda}}^{1/2} \underline{\underline{U}} \langle \underline{q}\underline{q}^T \rangle \underline{\underline{U}}^T \underline{\underline{\Lambda}}^{1/2} = \underline{\underline{E}} \qquad /A.7.5/$$

i.e. the components of $\underline{r}$ are independent and N(0,1). Eq. /A.7.3/ gives the following expression for q_1:

$$q_1 = \sigma^2\sqrt{2} \sum_{\ell=1}^{L} U_{1\ell} r_\ell / \sqrt{\lambda_\ell} \qquad /A.7.6/$$

where $u_{1\ell}$ is an element of matrix $\underline{\underline{U}}$ and λ_ℓ a diagonal element of the diagonal matrix $\underline{\underline{\Lambda}}$. Putting our previous results in eq. /IV.2.14/, we obtain

$$\frac{1}{\sigma^4} T_{min} = \sum_{\ell=1}^{L} r^2 - \frac{(\sum_{\ell=1}^{L} U_{1\ell} r_\ell / \sqrt{\lambda_\ell})^2}{n_1 - m} \ . \qquad /A.7.7/$$

As in Appendix 3, we introduce a new orthogonal transformation $\underline{\underline{A}}$:

$$\underline{z} = \underline{\underline{A}}\ \underline{r} \qquad /A.7.8/$$

the first row of which is

$$z_1 = \frac{1}{\sqrt{n_1 - m}} \sum_{\ell=1}^{L} U_{1\ell}\ r_\ell / \sqrt{\lambda_\ell} \quad . \qquad /A.7.9/$$

It is trivial that the components z_ℓ are independent from each other and are N(0,1). Eq. /A.7.7/ is now rewritten as

$$\frac{1}{\sigma^4} T_{min} = \sum_{\ell=1}^{L} z_\ell^2 - z_1^2 = \sum_{\ell=2}^{L} z_\ell^2 = \chi^2_{L-1} \qquad /A.7.10/$$

which proves eq. /IV.2.15/.

Comparison of eqs. /A.7.6/ and /A.7.9/ shows that

$$z_1 = \frac{q_1}{\sigma^2 \sqrt{2(n_1 - m)}} \quad . \qquad /A.7.11/$$

According to eq. /A.7.10/, z_1 does not occur in the sum giving T_{min}/σ^4 therefore, z_1 and T_{min} are independent, and so are q_1 and T_{min}.

This proof may be simply generalized to the case of eq. /IV.2.18/. As all summations go from k to L in eq. /IV.2.17/, we may carry out a change of subscripts: we assign subscript 1 to ℓ=k, subscript 2 to ℓ=k+1, and so on; finally ℓ=L gets the subscript (L-k+1). The same change of subscripts is possible for matrix $(\underline{\underline{S}}^k)^{-1}$ defined by eq. /IV.2.6a/. In this way, the problem is reduced to the proof of eq. /IV.2.15/. Since the role of L is now played by (L-k+1), we have from eq. /A.7.10/ that

$$T_k = \sigma^4 \chi^2_{L-k} \quad . \qquad /A.7.12/$$

The role of Q_1 is played by Q_k, consequently, T_k and Q_k are independent.

An algorithm analogous to that described in Appendix 5 may be derived for the computation of T_k. As in Appendix 5, define

$$z_\ell = \sum_{\ell'=k}^{L} S^k_{\ell\ell'} (Q_{\ell'} - \tilde{\sigma}_k (n_{\ell'} - m)) \qquad /A.7.13/$$

where $\tilde{\sigma}_k^2$ is given by eq. /IV.2.16/. Then, according to eq. /IV.2.10/,

$$T_k = \frac{1}{2} \sum_{\ell=k}^{L} z_\ell (Q_\ell - \tilde{\sigma}_k^2 (n_\ell - m)) \quad . \qquad /A.7.14/$$

From the definition of matrix $\underline{\underline{S}}^k$ given in eq. /IV.2.6a/, z_ℓ satisfies the following set of equations:

$$\text{for } \ell = k: \quad \sum_{\ell'=k}^{L} z_{\ell'}(n_{\ell'}-m) = Q_k - \tilde{\sigma}_k^2(n_k-m) = 0 \qquad /A.7.15a/$$

for $k<\ell\leq L$:

$$(n_\ell-m)\sum_{\ell'=k}^{\ell-1} z_{\ell'} + \sum_{\ell'=\ell}^{L} z_{\ell'}(n_{\ell'}-m) = Q_\ell - \tilde{\sigma}_k^2(n_\ell-m). \qquad /A.7.15b/$$

By analogy with eq. /A.5.5/, we set now

$$\mu_\ell = \sum_{\ell'=\ell}^{L} z_{\ell'}(n_{\ell'}-m) \qquad /A.7.16/$$

and

$$z_\ell = \begin{cases} \dfrac{\mu_\ell - \mu_{\ell+1}}{n_\ell - m} & \text{if} \quad \ell \leq L-1 \\ \dfrac{\mu_L}{n_L - m} & \text{if} \quad \ell = L \end{cases} \qquad /A.7.17/$$

From eq. /A.7.15a/, it follows that

$$\mu_k = 0 \; . \qquad /A.7.18/$$

Eq. /A.7.15b/ may be rewritten as

$$\sum_{\ell'=k}^{\ell-1} z_{\ell'} + \frac{\mu_\ell}{n_\ell - m} = \tilde{\sigma}_\ell^2 - \tilde{\sigma}_k^2 \; . \qquad /A.7.19/$$

Writing down this equation for $(\ell+1)$ and substracting eq. /A.7.19/ from it, we get

$$z_\ell + \frac{\mu_{\ell+1}}{n_{\ell+1}-m} - \frac{\mu_\ell}{n_\ell - m} = \frac{\mu_\ell - \mu_{\ell+1}}{n_\ell - m} + \frac{\mu_{\ell+1}}{n_{\ell+1}-m} - \frac{\mu_\ell}{n_\ell - m} = \tilde{\sigma}_{\ell+1}^2 - \tilde{\sigma}_\ell^2$$

or

$$\mu_{\ell+1} = \frac{\tilde{\sigma}_{\ell+1}^2 - \tilde{\sigma}_\ell^2}{\dfrac{1}{n_{\ell+1}-m} - \dfrac{1}{n_\ell - m}} \quad , \quad \ell \leq L-1 \qquad /A.7.20/$$

This is allowed to do for $\ell=k+1, k+2, \ldots, L-1$. We show that this is still valid even for $\ell=k$. Eq. /A.7.15b/ for $\ell=k+1$ may be put as

$$(n_{k+1}-m)z_k + \mu_{k+1} = Q_{k+1} - \tilde{\sigma}_k^2(n_{k+1}-m) \qquad /A.7.21/$$

Taking into account that $\mu_k=0$, we have from eq. /A.7.17/ that

$$z_k = -\frac{\mu_{k+1}}{n_k-m}$$

which in eq. /A.7.21/ yields

$$\mu_{k+1} = \frac{\tilde{\sigma}_{k+1}^2 - \tilde{\sigma}_k^2}{\frac{1}{n_{k+1}-m} - \frac{1}{n_k-m}} .$$

This is just what eq. /A.7.20/ results for $\ell=k$.

Inserting the z_ℓ calculated up to now in eq. /A.7.14/, we obtain

$$T_k = \frac{1}{2}\sum_{\ell=k}^{L} z_\ell Q_\ell - \frac{\tilde{\sigma}_k^2}{2}\sum_{\ell=k}^{L} z_\ell(n_\ell-m) = \frac{1}{2}\sum_{\ell=k}^{L} z_\ell Q_\ell .$$

Putting in here z_ℓ from eq. /A.7.17/, this goes over in

$$T_k = \frac{1}{2}\mu_L \frac{Q_L}{n_L-m} + \frac{1}{2}\sum_{\ell=k}^{L-1}(\mu_\ell-\mu_{\ell+1})\tilde{\sigma}_\ell^2 .$$

Using here the identity

$$(\mu_\ell-\mu_{\ell+1})\tilde{\sigma}_\ell^2 = \mu_\ell\tilde{\sigma}_\ell^2 - \mu_{\ell+1}\tilde{\sigma}_{\ell+1}^2 + \mu_{\ell+1}(\tilde{\sigma}_{\ell+1}^2 - \tilde{\sigma}_\ell^2),$$

we get that

$$T_k = \frac{1}{2}\sum_{\ell=k}^{L-1}\mu_{\ell+1}(\tilde{\sigma}_{\ell+1}^2 - \tilde{\sigma}_\ell^2) = \sum_{\ell=k}^{L-1}\frac{(\tilde{\sigma}_{\ell+1}^2 - \tilde{\sigma}_\ell^2)^2}{\frac{2}{n_{\ell+1}-m} - \frac{2}{n_\ell-m}} .$$

Thus, we obtained finally that

$$T_k = \sum_{\ell=k}^{L-1} u_\ell^2 \qquad /A.7.22/$$

where

$$u_\ell = \frac{\tilde{\sigma}_{\ell+1}^2 - \tilde{\sigma}_\ell^2}{\sqrt{\frac{2}{n_{\ell+1}-m} - \frac{2}{n_\ell-m}}} . \qquad /A.7.23/$$

Using eqs. /IV.2.4/ and /IV.2.5/, it is straightforward to show that u_ℓ is $N(0,\sigma^2)$ and they are uncorrelated.

Eqs. /A.7.22/ and /A.7.23/ provide a very convenient way for calculating T_k. These results, however, represent much more than a mere computational facility. First, they provide an alternative proof of eq. /IV.2.18/. Furthermore, they may be made the basis of a stepwise test for the asymptoticity of Q_k.

We know that T_k and Q_k are independent. Q_k does not occur at all in the expression of T_{k+1} /see eq. /IV.2.17//. Consequently, Q_k is independent of $u_k^2 = T_k - T_{k+1}$. We form the quotient

$$\vartheta_k = \frac{u_k}{Q_k/(n_k-m)} = \frac{\xi}{\chi^2_{n_k-m}/(n_k-m)} \qquad /A.7.24/$$

which is similar to the Student fraction /the square root is missing in the denominator/ and may be used for tests analogous to the Student test. The quantiles of ϑ_k are identical with the quantiles of $\varphi_{n_k-m,1}$ defined in eq./A.2.1/.

APPENDIX 8.

THE STATISTICAL PROPERTIES OF y_i^n

By differentiating eq. /V.2.4/, it may be simply shown that

$$< y_i^n> = \frac{<y_i>}{<a_{j+m_o}>} - \frac{<\Delta y_i \Delta a_{j+m_o}> - <(\Delta a_{j+m_o})^2>}{a_{j+m_o}^2} + \mathcal{O}(\sigma^4), \qquad /A.8.1/$$

consequently,

$$y_i^{n*} = y_i^n + \frac{<\Delta y_i \Delta a_{j+m_o}> - <(\Delta a_{j+m_o})^2>}{a_{j+m_o}^2} \qquad /A.8.2/$$

in unbiased i.e. its expectation is equal to $\psi(x_i, \underline{a}_o) + \mathcal{O}(\sigma^4)$. The standard deviation is given by

$$<\Delta y_i^n> = y_i^n \sqrt{\frac{<(\Delta y_i)^2>}{y_i^2} - 2\,\frac{<\Delta y_i \Delta a_{j+m_o}>}{y_i\, a_{j+m_o}} - \frac{<(\Delta a_{j+m_o})^2>}{a_{j+m_o}^2}} \qquad /A.8.3/$$

In order to use these formulae, we need the variances of y_i and a_{j+m_o} and their covariances. According to eq. /I.2.3/,

$$<(\Delta y_i)^2> = \frac{\sigma^2}{W_i} \qquad /A.8.4/$$

while from eq. /II.1.13/,

$$<(\Delta a_{j+m_o})^2> = \sigma^2 \{\underline{\underline{M}}^{-1}\}_{j+m_o, j+m_o} \qquad /A.8.5/$$

It may shown by using eq. /II.1.12/ that

$$<\Delta y_i \Delta a_{j+m_o}> = \sigma^2 \{\underline{\underline{M}}^{-1}\, \underline{f}_i\}_{j+m_o} = \sigma^2 \sum_{k=1}^{J+m_o} \{\underline{\underline{M}}^{-1}\}_{k, j+m_o} F_{ki} \qquad /A.8.6/$$

where $\underline{f}_i^T$ is the i^{th} row of matrix $\underline{\underline{F}}$.

As to these error formulae, it is noted that the covariance term gives a very small contribution in eq. /A.8.3/ in most practical cases. Similarly, the bias term in eq. /A.8.1/ is also very small so that y_i^n may be used as the normalized distribution in a very good approximation.

APPENDIX 9.

SOLUTION OF THE SET OF EQUATIONS /V.2.15/, /V.2.16/

The form of the set of equations /V.2.15/-/V.2.16/ suggests the following iterative method. Setting $\tilde{\Psi}_I \equiv 1$ for all I as an initial guess, eq. /V.2.15/ yields the first iterate for $\tilde{a}_j$ which in eq. /V.2.16/ gives the new iterate for $\tilde{\Psi}_I$ and so on. We have to study first under which conditions this procedure converges.

Denoting the solution by $\tilde{\Psi}_I$ and $\tilde{a}_j$, an iterate may be written as

$$a_j = \tilde{a}_j(1+A_j), \qquad /A.9.1a/$$

$$\Psi_I = \tilde{\Psi}_I(1+f_I). \qquad /A.9.1b/$$

Inserting this in eq. /V.2.15/, and keeping only first powers of A_j and f_I, we get

$$\tilde{a}_j(A_j+1) = \frac{\sum_{i\epsilon R_j} W_i(y_i-\alpha_i)\tilde{\Psi}_{I_i}(1+f_{I_i})\mu_i}{\sum_{i\epsilon R_j} W_i[\tilde{\Psi}_{I_i}(1+f_{I_i})\mu_i]^2} \approx$$

$$\approx \tilde{a}_j + \frac{\sum_{i\epsilon R_j} W_i(y_i-\alpha_i-\tilde{a}_j\tilde{\Psi}_{I_i}\mu_i)\tilde{\Psi}_{I_i}\mu_i f_{I_i} - \tilde{a}_j \sum_{i\epsilon R_j} W_i(\tilde{\Psi}_{I_i}\mu_i)^2 f_{I_i}}{\sum_{i\epsilon R_j} W_i(\tilde{\Psi}_{I_i}\mu_i)^2}$$

In the first sum of the nominator $(y_i-\alpha_i-a_j\tilde{\Psi}_{I_i}\mu_i)$ is small as compared to $\tilde{a}_j\tilde{\Psi}_{I_i}\mu_i$ /these two factors make the difference of the sums in the nominator/ so that the first sum may be neglected. Consequently, in first approximation

$$A_j = -\frac{\sum_{i\epsilon R_j} W_i(\tilde{\Psi}_{I_i}\mu_i)^2 f_{I_i}}{\sum_{i\epsilon R_j} W_i(\tilde{\Psi}_{I_i}\mu_i)^2} = -\sum_{I=1}^{N} D_{jI} f_I \qquad /A.9.2/$$

where

$$D_{jI} = \frac{\sum_{i\in R_j, x_i=r_I} W_i(\tilde{\psi}_{I_i}\mu_i)^2}{\sum_{i\in R_j} W_i(\tilde{\psi}_{I_i}\mu_i)^2} .$$

From this definition, it follows that

$$\sum_{I=1}^{N} D_{jI} = 1 . \qquad /A.9.3/$$

In a completely analogous way, we derive that

$$f_I = - \sum_{j=1}^{J} C_{Ij} A_j \qquad /A.9.4/$$

$$C_{Ij} = \frac{\sum_{i\in R_j, x_i=r_I} W_i(\hat{a}_j\mu_i)^2}{\sum_{j=1}^{J} \sum_{i\in R_j, x_i=r_I} W_i(\hat{a}_j\mu_i)^2} .$$

It may be stated for these coefficients as well that

$$\sum_{j=1}^{J} C_{Ij} = 1 . \qquad /A.9.5/$$

If we compose vectors $\underline{A}$ and $\underline{f}$ from the A_j and f_I as components, and matrices $\underline{\underline{C}}$ and $\underline{\underline{D}}$ from the elements C_{Ij} and D_{jI}, eqs. /A.9.2/ and /A.9.4/ may be put as

$$\underline{A} = - \underline{\underline{D}}\, \underline{f}$$

and

$$\underline{f} = - \underline{\underline{C}}\, \underline{A} .$$

Let us denote the ℓ^{th} iterates by $\underline{f}_\ell$ and $\underline{A}_\ell$, then these equations lead to the following iteration scheme:

$$\underline{A}_{\ell+1} = - \underline{\underline{D}}\, \underline{f}_\ell \qquad /A.9.6/$$

$$\underline{f}_{\ell+1} = - \underline{\underline{C}}\, \underline{A}_{\ell+1} = \underline{\underline{C}}\, \underline{\underline{D}}\, \underline{f}_\ell = \underline{\underline{\Omega}}\, \underline{f}_\ell \qquad /A.9.7/$$

Taking into account that the elements of $\underline{\underline{\Omega}}$ are given by

$$\Omega_{II'} = \sum_{j=1}^{J} C_{Ij} D_{jI'} \qquad /A.9.8/$$

it may be shown that the rows of $\underline{\underline{\Omega}}$ are also normalized to 1:

$$\sum_{I'=1}^{N} \Omega_{II'} = 1 . \qquad /A.9.9/$$

It is known from the theory of iteration schemes like eq. /A.9.7/ that the convergence depends on the largest eigenvalue λ_m of matrix $\underline{\underline{\Omega}}$. After a sufficiently large number of iteration steps, $\underline{f}_\ell$ is proportional to the eigenvector $\underline{e}_m$ corresponding to λ_m. Then each iteration step results in a multiplication by λ_m:

$$\underline{f}_\ell \approx \omega \lambda_m^\ell \underline{e}_m \qquad /A.9.10/$$

where ω is some constant depending only on $\underline{f}_o$ i.e. on the initial guess. Consequently, $\underline{f}_\ell$ tends to zero if $|\lambda_m|<1$, while the iteration is divergent if $|\lambda_m|>1$. Now, eq. /A.9.9/ assures that $|\lambda_m| \leq 1$. In order to show this, let us consider some eigenvalue λ and the related eigenvector $\underline{e}$. Suppose that e_I has the largest absolute value from among its components. Write down the eigenvalue equation for this I:

$$\sum_{I'=1}^{N} \Omega_{II'} e_{I'} = \lambda e_I$$

from which we obtain that

$$|\lambda| = \left| \sum_{I'=1}^{N} \Omega_{II'} \frac{e_{I'}}{e_I} \right| \leq \sum_{I'=1}^{N} \Omega_{II'} \left| \frac{e_{I'}}{e_I} \right| \leq \sum_{I'=1}^{N} \Omega_{II'} = 1 \qquad /A.9.11/$$

where it was taken into account that all elements of $\underline{\underline{\Omega}}$ are positive. We conclude that the iteration can not diverge. The equality can hold in eq. /A.9.11/ only if $e_{I'}/e_I=1$ for all I' . It follows from eq. /A.9.9/ that $e_I \equiv 1$ really is an eigenvector with $\lambda=1$ as the related eigenvalue. Consequently,

$$\lambda_m=1 \text{ and } e_{mI}=1, \quad I=1,2,\ldots,N.$$

This means that the the iteration converges to $f_I \equiv \omega$ and $A_j=-\omega$ /See eq. /A.9.2// or in terms of a_j and ψ_I , to

$$\Psi_I = \tilde{\Psi}_I(1+\omega)$$

$$a_j = \tilde{a}_j(1-\omega) \approx \frac{a_j}{1+\omega}$$

which is as good a solution of eqs. /V.2.15/ and /V.2.16/ as $\tilde{\Psi}_I$ and $\tilde{a}_j$.

We have found that the iteration converges but the result is indefinite up to a factor of proportionality. The convergence rate is determined by the largest such eigenvalue for which $|\lambda|<1$. We do not study how large it is.

In order to make the solution definite, it is advisable to fix one of the unknowns or a linear combination of them. Since one is mainly interested in the distribution, we fix that

$$\sum_{I=1}^{N} S'_I \Psi_I = 1 \qquad /A.9.12/$$

or, in terms of f_I:

$$\sum_{I=1}^{N} S_I f_I = 0 \quad , \quad S_I = S'_I \tilde{\Psi}_I \qquad /A.9.13/$$

where, according to eq. /A.9.12/,

$$\sum_{I=1}^{N} S_I = 1 \; . \qquad /A.9.14/$$

Now, we may assure the validity of eq. /A.9.12/ for example in such a way that each iterate is divided by the sum

$$\sum_{I=1}^{N} S'_I \Psi_{I\ell} .$$

It may be simply shown that this division is equivalent to the substraction of

$$\sum_{I=1}^{N} S_I \underline{f}_{I\ell}$$

from each of the $f_{I\ell}$. If $\underline{S}$ is considered as a vector with components S_I and $\underline{e}$ is a vector all components of which are equal to 1, such a procedure corresponds to the following iteration scheme instead of /A.9.7/:

$$\underline{f}_{\ell+1} = \underline{\underline{\Omega}} \underline{f}_\ell - \underline{e}\, \underline{S}^T \underline{\underline{\Omega}} \underline{f}_\ell = (\underline{\underline{E}} - \underline{e}\, \underline{S}^T)\, \underline{\underline{\Omega}} \underline{f}_\ell \; . \qquad /A.9.15/$$

In these notations, eq. /A.9.14/ may be put as

$$\underline{S}^T \underline{e} = 1 \; . \qquad /A.9.16/$$

Consequently, the iteration matrix of this procedure is

$$\underline{\underline{T}} = (\underline{\underline{E}} - \underline{e}\, \underline{s}^T)\, \underline{\underline{\Omega}} \; . \qquad /A.9.17/$$

We have seen above that $\underline{e}$ is an eigenvector of $\underline{\underline{\Omega}}$ corresponding to the eigenvalue $\lambda=1$. Therefore, we get from eq. /A.9.16/ and /A.9.17/ that

$$\underline{\underline{T}}\, \underline{e} = 0.$$

This mean that, already in the first iteration, this eigenvector dies out, and only those remain for which $|\lambda|<1$. It may be shown, however, that these ones do not die out faster than without assuring the validity of eq. /A.9.12/ in each step. In fact, if eigenvector $\underline{u}$ corresponds to eigenvalue λ, i.e.

$$\underline{\underline{\Omega}}\ \underline{u} = \lambda \underline{u}\ ,$$

a direct substitution shows that this λ is an eigenvalue also of $\underline{\underline{T}}$:

$$\underline{\underline{T}}(\underline{u}-\underline{\underline{e}}\underline{S}^T\underline{u}) = \lambda(\underline{u}-\underline{\underline{e}}\underline{S}^T\underline{u}). \qquad /A.9.18/$$

We may conclude that the eigenvalues are not changed by condition /A.9.12/. This entails also that it is fully sufficient to take condition /A.9.12/ into account after convergence.

The eigenvalues may be reduced by an overrelaxation procedure. It is straightforward to show that, if the overrelaxation factor is β, the corresponding iteration matrix is

$$\underline{\underline{T}}(\beta) = \beta(\underline{\underline{E}}-\underline{\underline{e}}\underline{S}^T)\ \underline{\underline{\Omega}} + (1-\beta)\ \underline{\underline{E}} \qquad /A.9.19/$$

and eigenvalue λ is changed to

$$\lambda(\beta) = 1-\beta(1-\lambda). \qquad /A.9.20/$$

The corresponding eigenvector dies out in one iteration step if

$$\beta = \frac{1}{1-\lambda}. \qquad /A.9.21/$$

This shows that the optimum value of β depends on which eigenvector predominates in the actual stage of the iteration. We do not go into further details of this.

APPENDIX 10.

LIST OF NUMERICAL EXAMPLES

The numerical examples treated in this paper are "measured" values simulated by a random number generator. All values are sampled from the Poissonian distribution. In the following list, the mean values $\langle y_i \rangle$ are given. In all cases,

$$x_i = x_1 + (i-1)\Delta x$$

where

$$x_1 = \Delta x = 1.$$

The total number of points is always n=100.

Case 1 $\quad \langle y_i \rangle = a_1[\cos a_2(x_i - a_3)]$

$$a_1 = 10^4 \quad , \quad a_2 = 0.02 \quad , \quad a_3 = 30 \; .$$

Case 2 As in case 1 but $a_1 = 10^3$

Case 3 As in case 1 but $a_1 = 10^2$

Case 4 $\quad \langle y_i \rangle = a_1 e^{-a_2 x_i} + a_3$

$$a_1 = 10^4 \quad , \quad a_2 = 0{,}1 \quad , \quad a_3 = 10^3$$

Case 5

$$\langle y_i \rangle = \begin{cases} a_1 \cos[a_2(x_i - a_3)] & \text{for } x_i \leq 20 \text{ and } x_i \geq 28 \\ a_1 \cos[a_2(x_i - a_3)] - \frac{a_1}{10}\left[1 - \frac{(x_i-24)^2}{16}\right] & \text{for } 21 \leq x_i \leq 27 \end{cases}$$

$$a_1 = 10^4 \quad , \quad a_2 = 0{,}02 \quad , \quad a_3 = 30 \; .$$

Case 6 As in case 5 but $a_1 = 10^3$

Case 7 $\quad \langle y_i \rangle = a_1[\cos(a_2(x_i - a_3)) + a_4 \operatorname{ch}(a_5(x_i - a_3))]$

$$a_1 = 10^4 \quad , \quad a_2 = 0{,}02 \; , \quad a_3 = 30 \; , \; a_4 = 5 \cdot 10^{-6} \; , \; a_5 = 0.17$$

Case 8 As in case 7 but $a_1 = 10^3$

Case 9 As in case 7 but $a_4 = 3 \cdot 10^{-6}$, $a_5 = 0.16$

Case 10 $\langle y_i \rangle = a_1(e^{-a_2 x_i} + a_3 e^{-a_4 x_i}) + a_5$

$a_1 = 10^4$, $a_2 = 0.1$, $a_3 = 0.5$, $a_4 = 0.4$, $a_5 = 10^3$

Case 11

$$\langle y_i \rangle = \begin{cases} a_3 \cos[a_1(x_i - a_2)] & \text{for } x_i \leq 32 \\ a_4 \cos[a_1(x_i - a_2)] & \text{for } 33 \leq x_i \leq 66 \\ a_5 \cos[a_1(x_i - a_2)] & \text{for } 67 \leq x_i \leq 100 \end{cases}$$

$a_1 = 0.02$, $a_2 = 30$, $a_3 = 2 \cdot 10^4$, $a_4 = 10^4$, $a_5 = 3 \cdot 10^4$.

APPENDIX 11.

THE STATISTICAL PROPERTIES OF THE t_i FRACTIONS

All fractions t_i have the same distribution function. It may be derived using eq. /III.2.9/. t_i' is a Student fraction with the density

$$s_{n-m-1}(x) = \frac{1}{\sqrt{\pi(n-m-1)}} \frac{\Gamma(\frac{n-m}{2})}{\Gamma(\frac{n-m-1}{2})} (1 + \frac{x^2}{n-m-1})^{-\frac{n-m}{2}} \qquad /A.11.1/$$

/see /2//. Using eq. /III.2.9/ we may put that

$$P\{t_i<z\} = P\{t_i'< \frac{z}{\sqrt{1-\frac{z^2-1}{n-m-1}}}\} = \int_{-\infty}^{z/\sqrt{1-\frac{z^2-1}{n-m-1}}} s_{n-m-1}(x)dx \ .$$

Differentiation by z leads to the probability density function of t_i:

$$f_{n-m}(x) = \frac{1}{\sqrt{\pi(n-m)}} \frac{\Gamma(\frac{n-m}{2})}{\Gamma(\frac{n-m-1}{2})} (1 - \frac{x^2}{n-m})^{\frac{n-m-3}{2}} \qquad /A.11.2/$$

Figure A.2 shows a comparison of these two distributions for some values of (n-m). Although these curves are quite similar for n-m>10, quantiles γ and γ' are sensibly different as Table A.1 shows. It is yet interesting to note that the variance of t_i is 1 for all (n-m) while that of t_i' is (n-m-1)/(n-m-3) for (n-m)>3 /it does not exist for (n-m)$\leq$3/.

As to the collective behaviour of the t_i for inner points, things are a little more complicated. The first interesting property is that they are not linearly independent. Indeed, we show that m out of all t_i can be expressed as linear combinations of the others /see also ref [2]/. From this point of view, it is sufficient to consider the components of vector $(\underline{y}-\tilde{\underline{y}})$ which was obtained in eq. /II.5.1/ as

$$\underline{y}-\tilde{\underline{y}} = (\underline{\underline{E}}-\underline{\underline{F}}\underline{\underline{M}}^{-1}\underline{\underline{F}}^T\underline{\underline{W}})\Delta\underline{y} \ .$$

This may be rewritten as

$$\underline{\underline{W}}^{1/2}(\underline{Y}-\tilde{\underline{Y}}) = (\underline{\underline{E}}-\underline{\underline{A}})\ \underline{\underline{W}}^{1/2}\ \Delta\underline{Y} \qquad /A.11.3/$$

where

$$\underline{\underline{A}} = \underline{\underline{W}}^{1/2}\ \underline{\underline{F}}\ \underline{\underline{M}}^{-1}\ \underline{\underline{F}}^{T}\ \underline{\underline{W}}^{1/2}\ . \qquad /A.11.4/$$

It follows from eq. /II.1.3/ that all components of vector $\underline{\underline{W}}^{1/2}\Delta\underline{Y}$ are $N(0,\sigma)$ and they are statistically independent. It may be directly verified that matrix $\underline{\underline{A}}$ is a projector i.e. it satisfies the matrix equation

$$\underline{\underline{A}}^{2} = \underline{\underline{A}}\ . \qquad /A.11.5/$$

Now, if the eigenvalues of $\underline{\underline{A}}$ are denoted by λ_i , it follows from this that

$$\lambda_i = 0 \quad \text{or} \quad 1. \qquad i = 1,2,\ldots,n \qquad /A.11.6/$$

The number of $\lambda_i = 1$ is equal to rank($\underline{\underline{A}}$). We prove that

$$\text{rank}(\underline{\underline{A}}) = m\ . \qquad /A.11.7/$$

It was assumed that $\underline{\underline{M}}^{-1}$ exists /otherwise the fitting can not be carried out/, therefore, $\text{rank}(\underline{\underline{W}}^{1/2}\ \underline{\underline{F}}) = \text{rank}(\underline{\underline{M}}) = m$. The rank cannot increase by matrix multiplication so that we obtain from eq. /A.11.4/ that

$$\text{rank}(\underline{\underline{A}}) \leq m\ . \qquad /A.11.8a/$$

Taking into account eqs. /II.1.4/ and /A.11.4/, we get that

$$\underline{\underline{F}}^{T}\ \underline{\underline{W}}^{1/2}\ \underline{\underline{A}} = \underline{\underline{F}}^{T}\ \underline{\underline{W}}^{1/2}\ ,$$

consequently,

$$\text{rank}(\underline{\underline{A}}) \geq m\ . \qquad /A.11.8b/$$

Formulae /A.11.8/ can be valid only if eq. /A.11.7/ holds.

There exists an orthogonal matrix $\underline{\underline{U}}$ such that

$$\underline{\underline{A}} = \underline{\underline{U}}^{T}\ \underline{\underline{\Lambda}}\underline{\underline{U}} \qquad /A.11.9/$$

where $\underline{\underline{\Lambda}}$ is a diagonal matrix with λ_i in the main diagonal. Putting this in eq. /A.11.3/, we get

$$\underline{\underline{U}}\ \underline{\underline{W}}^{1/2}(\underline{Y}-\tilde{\underline{Y}}) = (\underline{\underline{E}}-\underline{\underline{\Lambda}})\underline{\underline{U}}\underline{\underline{W}}^{1/2}\Delta\underline{Y}\ . \qquad /A.11.10/$$

The elements of diagonal matrix $(\underline{\underline{E}}-\underline{\underline{\Lambda}})$ are equal to $(1-\lambda_i)$ which are also equal to 0 or 1. It follows from eq. /A.11.7/ that the number of elements which are 0 is m. Suppose that subscripts i are ordered such that

$$1 - \lambda_i = 0 \qquad \text{for} \quad i=1,2,\ldots,m.$$

Then it follows from eq. /A.11.10/ that

$$\sum_{i=1}^{n} \{\underline{\underline{U}}\ \underline{\underline{W}}^{1/2}\}_{ji}\ (y_i - \tilde{y}_i) = 0 \quad \text{for} \quad j=1,2,\ldots,m$$

/A.11.11/

This means that m out of the $(y_i - \tilde{y}_i)$ may really be expressed as linear combinations of the others as stated above.

When the collective behaviour of the $(y_i - \tilde{y}_i)$ are studied, it must be taken into account that only (n-m) out of them bear linearly independent statistical information. Of course, these linearly independent components are not statistically independent. Their distribution is given by the (n-m) dimensional normal distribution. Their covariance matrix could be formally obtained from eq. /A.11.10/ but we do not go into further details because we would not get far in such a full generality.

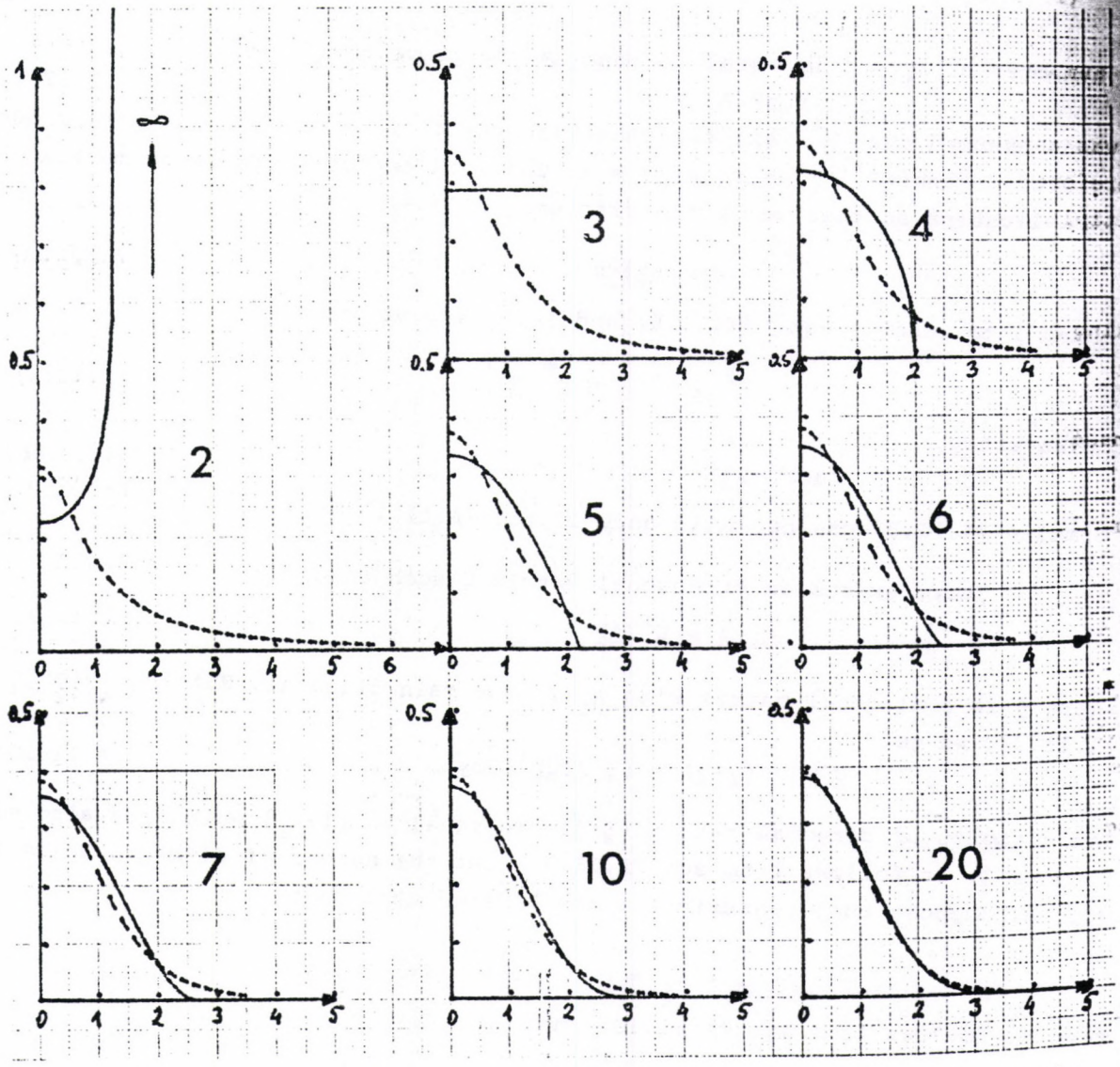


Fig. A.2 Comparison of the Student distribution /dotted line/ with the distribution of t_i /continuous line/ for some values of /n-m/

APPENDIX 12

EXPECTATION AND VARIANCE OF COUNTS WITH DEAD TIME LOSSES

It is derived in ref. [1] that the exact Laplace transform of $P_k(\tau,T)$ given in eq. /I.2.16/ with respect to T is

$$P_k(v) = \int_0^\infty P_k(\tau,T)e^{-vT}\,dT = \frac{\lambda}{v(\lambda+v)}\left(1-\frac{\lambda e^{-vT}}{\lambda+v}\right)\left(\frac{\lambda e^{-vT}}{\lambda+v}\right)^{k-1} \qquad /A.12.1/$$

for $k \geq 1$ and

$$P_o(v) = \frac{1}{\lambda+v} \quad . \qquad /A.12.2/$$

It may be simply shown that the Laplace transforms of the first and second moments $m_1(v)$ and $m_2(v)$, resp., of this distribution are

$$m_1(v) = \frac{1}{v}\,\frac{1}{v+\lambda(1-e^{-v\tau})} \quad , \qquad /A.12.3/$$

$$m_2(v) = \frac{\lambda}{v}\,\frac{v+\lambda\ 1+e^{-v\tau}}{[v+\lambda(1-e^{v\tau})]^2} \quad . \qquad /A.12.4/$$

The inverse transforms of these expressions may be obtained by the well known formulae

$$m_1(T) = \sum_n \operatorname{rez}\left[m_1(v)e^{vT}\right]_{v=v_n} \qquad /A.12.5/$$

$$m_2(T) = \sum_n \operatorname{rez}\left[m_2(v)e^{vT}\right]_{v=v_n} \qquad /A.12.6/$$

The functions $m_1(v)$ and $m_2(v)$ have the following singularities:

a/ $v=0$, second order for $m_1(v)$ and third order for $m_2(v)$,

b/ $v_n=z_n/\tau\ (n=1,2,\ldots)$ where the z_n are the roots of

$$H(z) = z + \lambda\tau(1-e^{-z}) = 0.$$

The residuals for v=0 may be calculated in a straightforward way as

$$\text{rez}\left[m_1(v)e^{vT}\right]_{v=0} = \frac{\lambda T}{1+\lambda\tau} + \frac{(\lambda\tau)^2/2}{(1+\lambda\tau)^2} \qquad /A.12.7/$$

and

$$\text{rez}\left[m_2(v)e^{vT}\right]_{v=0} = \left(\frac{\lambda T}{1+\lambda\tau}\right)^2 + \frac{\lambda T}{(1+\lambda\tau)^3} + \frac{\lambda^2\tau^2}{(1+\lambda\tau)^3} + \frac{\lambda^2\tau^2(1/2+\lambda^2\tau^2)}{(1+\lambda\tau)^4} - \frac{2\lambda^3\tau^3/3}{(1+\lambda\tau)^3}. \qquad /A.12.8/$$

The real parts of the z_n are negative and it may be shown by numerical calculations that, for realistic values of $\lambda\tau$, they are less than -1. Taking into account that these roots lead to residuals proportional to exp $\{z_n T/\tau\}$, they may surely be neglected because $T/\tau \gg 1$. In such a way, we obtained for the expectation

$$m_1(T) = \frac{\lambda T}{1+\lambda\tau} \qquad /A.12.9/$$

and for the variance

$$\sigma^2(T) = m_2(T) - \left[m_1(T)\right]^2 = \frac{\lambda T}{(1+\lambda\tau)^3}, \qquad /A.12.10/$$

if terms of the order $(\lambda\tau)^2$ and higher are neglected.

able A.1

The values of the Student quantiles γ and the quantiles of the modified Student distribution γ'

They are defined by the equations /III.1.3/ and /III.2.11/.

STUDENT AND MODIFIED STUDENT QUANTILES
(N DEGREES OF FREEDOM)

	EPS=0.010		EPS=0.050	
N	STUDENT	MODIFIED	STUDENT	MODIFIED
1	63.6567		12.7062	
2	9.9248	1.4140	4.3027	1.4099
3	5.8409	1.7147	3.1824	1.6454
4	4.6041	1.9175	2.7764	1.7567
5	4.0321	2.0509	2.5706	1.8143
6	3.7074	2.1421	2.4469	1.8481
7	3.4995	2.2075	2.3646	1.8698
8	3.3554	2.2562	2.3060	1.8848
9	3.2498	2.2938	2.2622	1.8957
10	3.1693	2.3236	2.2281	1.9039
12	3.0545	2.3932	2.1788	1.9318
14	2.9768	2.4186	2.1448	1.9352
16	2.9208	2.4376	2.1199	1.9378
18	2.8784	2.4525	2.1009	1.9400
20	2.8453	2.4644	2.0860	1.9417
25	2.7874	2.5112	2.0595	1.9588
30	2.7500	2.5178	2.0423	1.9565
35	2.7238	2.5236	2.0301	1.9556
40	2.7045	2.5285	2.0211	1.9555
45	2.6896	2.5326	2.0141	1.9552
50	2.6778	2.5361	2.0086	1.9552
55	2.6682	2.5391	2.0040	1.9553
60	2.6603	2.5417	2.0003	1.9555
65	2.6536	2.5440	1.9971	1.9557
70	2.6479	2.5460	1.9944	1.9558
75	2.6430	2.5478	1.9921	1.9560
80	2.6387	2.5493	1.9901	1.9561
85	2.6349	2.5507	1.9883	1.9563
90	2.6316	2.5520	1.9867	1.9564
95	2.6286	2.5531	1.9853	1.9566
100	2.6259	2.5542	1.9840	1.9567
110	2.6213	2.5562	1.9818	1.9580
120	2.6174	2.5594	1.9799	1.9580
130	2.6142	2.5604	1.9784	1.9581
140	2.6114	2.5614	1.9771	1.9581
150	2.6090	2.5622	1.9759	1.9582
160	2.6069	2.5629	1.9749	1.9582
170	2.6051	2.5636	1.9740	1.9583
180	2.6034	2.5642	1.9732	1.9583
190	2.6020	2.5647	1.9725	1.9584
200	2.6006	2.5652	1.9719	1.9584
210	2.5994	2.5657	1.9713	1.9585
220	2.5984	2.5661	1.9708	1.9585
230	2.5974	2.5665	1.9703	1.9586
240	2.5965	2.5668	1.9699	1.9586

Table A.2

The values of the Fisher quantiles γ_f and φ-quantiles γ_φ

They are defined by the equations

$$P\left\{\frac{\chi_k^2/k}{\chi_\ell^2/\ell} < \gamma_f\right\} = 1-\varepsilon$$

and

$$P\left\{\frac{\chi_k/\sqrt{k}}{\chi_\ell^2/\ell} < \gamma_\varphi\right\} = 1-\varepsilon$$

STUDENT AND MODIFIED STUDENT QUANTILES
(N DEGREES OF FREEDOM)

	EPS=0.100		EPS=0.200	
N	STUDENT	MODIFIED	STUDENT	MODIFIED
1	6.3138		3.0777	
2	2.9200	1.3968	1.8856	1.3450
3	2.3534	1.5588	1.6377	1.3856
4	2.1318	1.6106	1.5332	1.3741
5	2.0150	1.6308	1.4759	1.3604
6	1.9432	1.6398	1.4398	1.3493
7	1.8946	1.6443	1.4149	1.3407
8	1.8595	1.6467	1.3968	1.3339
9	1.8331	1.6481	1.3830	1.3284
10	1.8125	1.6488	1.3722	1.3239
12	1.7823	1.6612	1.3562	1.3243
14	1.7613	1.6581	1.3450	1.3175
16	1.7459	1.6559	1.3368	1.3125
18	1.7341	1.6543	1.3304	1.3085
20	1.7247	1.6531	1.3253	1.3055
25	1.7081	1.6604	1.3163	1.3057
30	1.6973	1.6569	1.3104	1.3006
35	1.6896	1.6534	1.3062	1.2972
40	1.6839	1.6517	1.3031	1.2948
45	1.6794	1.6505	1.3006	1.2931
50	1.6759	1.6497	1.2987	1.2917
55	1.6730	1.6490	1.2971	1.2907
60	1.6706	1.6485	1.2958	1.2898
65	1.6686	1.6481	1.2947	1.2891
70	1.6669	1.6478	1.2938	1.2885
75	1.6654	1.6475	1.2929	1.2880
80	1.6641	1.6473	1.2922	1.2875
85	1.6630	1.6471	1.2916	1.2872
90	1.6620	1.6469	1.2910	1.2868
95	1.6611	1.6468	1.2905	1.2865
100	1.6602	1.6466	1.2901	1.2863
110	1.6588	1.6471	1.2893	1.2862
120	1.6577	1.6468	1.2886	1.2858
130	1.6567	1.6466	1.2881	1.2854
140	1.6558	1.6464	1.2876	1.2851
150	1.6551	1.6463	1.2872	1.2848
160	1.6544	1.6462	1.2869	1.2846
170	1.6539	1.6461	1.2866	1.2844
180	1.6534	1.6461	1.2863	1.2842
190	1.6529	1.6459	1.2860	1.2841
200	1.6525	1.6458	1.2858	1.2839
210	1.6521	1.6457	1.2856	1.2838
220	1.6518	1.6457	1.2854	1.2837
230	1.6515	1.6456	1.2852	1.2836
240	1.6512	1.6455	1.2851	1.2835

FISHER-QUANTILES EPS=0.010

L/K	1	2	3	4	5	6	7	8	9	10
12	9.3302	6.9266	5.9525	5.4120	5.0643	4.8206	4.6395	4.4994	4.3875	4.2961
14	8.8616	6.5149	5.5639	5.0354	4.6950	4.4558	4.2779	4.1399	4.0297	3.9394
16	8.5310	6.2262	5.2922	4.7726	4.4374	4.2016	4.0259	3.8896	3.7804	3.6909
18	8.2854	6.0129	5.0919	4.5790	4.2479	4.0146	3.8406	3.7054	3.5971	3.5082
20	8.0960	5.8489	4.9382	4.4307	4.1027	3.8714	3.6987	3.5644	3.4567	3.3682
25	7.7698	5.5680	4.6755	4.1774	3.8550	3.6272	3.4568	3.3239	3.2172	3.1294
30	7.5625	5.3903	4.5097	4.0179	3.6990	3.4735	3.3045	3.1726	3.0665	2.9791
35	7.4191	5.2679	4.3957	3.9082	3.5919	3.3679	3.2000	3.0687	2.9630	2.8758
40	7.3141	5.1785	4.3126	3.8283	3.5138	3.2910	3.1238	2.9930	2.8876	2.8005
45	7.2339	5.1103	4.2492	3.7674	3.4544	3.2325	3.0658	2.9353	2.8301	2.7452
50	7.1706	5.0566	4.1993	3.7195	3.4077	3.1864	3.0202	2.8900	2.7850	2.6981
55	7.1194	5.0132	4.1591	3.6809	3.3700	3.1493	2.9834	2.8534	2.7485	2.6617
60	7.0771	4.9774	4.1259	3.6490	3.3389	3.1187	2.9530	2.8233	2.7185	2.6318
65	7.0416	4.9474	4.0981	3.6223	3.3128	3.0930	2.9276	2.7980	2.6933	2.6066
70	7.0114	4.9219	4.0744	3.5996	3.2907	3.0712	2.9060	2.7765	2.6719	2.5852
75	6.9854	4.8999	4.0540	3.5801	3.2716	3.0524	2.8874	2.7580	2.6534	2.5668
80	6.9627	4.8807	4.0363	3.5631	3.2550	3.0361	2.8713	2.7420	2.6374	2.5508
85	6.9428	4.8639	4.0207	3.5482	3.2405	3.0218	2.8571	2.7279	2.6233	2.5368
90	6.9251	4.8491	4.0070	3.5350	3.2276	3.0091	2.8445	2.7154	2.6109	2.5243
95	6.9094	4.8358	3.9947	3.5232	3.2162	2.9978	2.8333	2.7042	2.5998	2.5132
100	6.8953	4.8239	3.9837	3.5127	3.2059	2.9877	2.8233	2.6943	2.5898	2.5033
110	6.8710	4.8035	3.9648	3.4946	3.1882	2.9703	2.8061	2.6771	2.5727	2.4862
120	6.8509	4.7865	3.9491	3.4795	3.1735	2.9559	2.7918	2.6629	2.5586	2.4721
130	6.8339	4.7722	3.9359	3.4669	3.1612	2.9437	2.7797	2.6509	2.5466	2.4602
140	6.8194	4.7600	3.9246	3.4561	3.1507	2.9333	2.7695	2.6407	2.5365	2.4500
150	6.8069	4.7495	3.9149	3.4467	3.1416	2.9244	2.7606	2.6319	2.5277	2.4412
160	6.7960	4.7403	3.9064	3.4386	3.1336	2.9166	2.7528	2.6242	2.5200	2.4335
170	6.7865	4.7322	3.8989	3.4314	3.1267	2.9097	2.7460	2.6174	2.5132	2.4268
180	6.7778	4.7250	3.8923	3.4251	3.1205	2.9036	2.7400	2.6114	2.5072	2.4208
190	6.7702	4.7186	3.8863	3.4194	3.1149	2.8982	2.7346	2.6061	2.5019	2.4154
200	6.7633	4.7129	3.8810	3.4143	3.1100	2.8933	2.7298	2.6012	2.4971	2.4106
250	6.7373	4.6911	3.8609	3.3950	3.0912	2.8748	2.7114	2.5830	2.4789	2.3925
300	6.7201	4.6766	3.8475	3.3823	3.0787	2.8625	2.6993	2.5709	2.4668	2.3804
350	6.7078	4.6663	3.8380	3.3732	3.0699	2.8538	2.6906	2.5625	2.4582	2.3718
400	6.6987	4.6586	3.8309	3.3664	3.0632	2.8472	2.6842	2.5559	2.4518	2.3654
450	6.6915	4.6526	3.8254	3.3611	3.0581	2.8422	2.6791	2.5509	2.4469	2.3604
500	6.6858	4.6478	3.8210	3.3569	3.0540	2.8381	2.6751	2.5469	2.4429	2.3565
550	6.6812	4.6439	3.8174	3.3534	3.0506	2.8348	2.6719	2.5436	2.4396	2.3532
600	6.6773	4.6407	3.8144	3.3505	3.0478	2.8321	2.6691	2.5409	2.4369	2.3505
650	6.6740	4.6380	3.8119	3.3481	3.0455	2.8297	2.6668	2.5386	2.4346	2.3482

FISHER-QUANTILES EPS=0.010

L/K	11	12	13	14	15	16	17	18	19	20
12	4.2198									
14	3.8640	3.8001	3.7452							
16	3.6162	3.5527	3.4981	3.4506	3.4089					
18	3.4338	3.3706	3.3162	3.2689	3.2273	3.1904	3.1575			
20	3.2941	3.2311	3.1769	3.1296	3.0880	3.0512	3.0183	2.9887	2.9620	
25	3.0558	2.9931	2.9389	2.8917	2.8502	2.8135	2.7803	2.7506	2.7238	2.6995
30	2.9057	2.8431	2.7890	2.7418	2.7002	2.6632	2.6301	2.6005	2.5732	2.5487
35	2.8026	2.7400	2.6859	2.6387	2.5970	2.5599	2.5266	2.4967	2.4695	2.4448
40	2.7274	2.6648	2.6107	2.5634	2.5216	2.4844	2.4511	2.4210	2.3937	2.3689
45	2.6701	2.6076	2.5534	2.5060	2.4642	2.4269	2.3935	2.3633	2.3359	2.3109
50	2.6250	2.5625	2.5083	2.4609	2.4190	2.3816	2.3481	2.3178	2.2903	2.2652
55	2.5887	2.5261	2.4719	2.4244	2.3824	2.3450	2.3114	2.2810	2.2535	2.2283
60	2.5587	2.4961	2.4419	2.3943	2.3523	2.3148	2.2811	2.2507	2.2230	2.1978
65	2.5335	2.4710	2.4167	2.3691	2.3270	2.2895	2.2557	2.2252	2.1975	2.1722
70	2.5122	2.4496	2.3953	2.3477	2.3055	2.2679	2.2341	2.2036	2.1758	2.1504
75	2.4938	2.4312	2.3768	2.3292	2.2870	2.2493	2.2155	2.1849	2.1571	2.1316
80	2.4777	2.4151	2.3608	2.3131	2.2709	2.2332	2.1993	2.1686	2.1408	2.1153
85	2.4637	2.4011	2.3467	2.2990	2.2567	2.2190	2.1851	2.1544	2.1264	2.1009
90	2.4513	2.3886	2.3342	2.2865	2.2442	2.2064	2.1725	2.1417	2.1137	2.0882
95	2.4402	2.3775	2.3231	2.2754	2.2330	2.1952	2.1612	2.1304	2.1024	2.0768
100	2.4302	2.3676	2.3132	2.2654	2.2230	2.1852	2.1511	2.1203	2.0923	2.0666
110	2.4132	2.3505	2.2960	2.2482	2.2058	2.1679	2.1338	2.1029	2.0748	2.0491
120	2.3990	2.3363	2.2818	2.2339	2.1915	2.1536	2.1194	2.0885	2.0604	2.0346
130	2.3871	2.3244	2.2698	2.2219	2.1795	2.1415	2.1073	2.0765	2.0481	2.0223
140	2.3769	2.3142	2.2596	2.2117	2.1692	2.1312	2.0970	2.0660	2.0377	2.0119
150	2.3681	2.3053	2.2508	2.2028	2.1603	2.1223	2.0880	2.0570	2.0287	2.0028
160	2.3604	2.2977	2.2431	2.1951	2.1526	2.1145	2.0802	2.0491	2.0208	1.9949
170	2.3537	2.2909	2.2363	2.1883	2.1457	2.1076	2.0733	2.0422	2.0139	1.9879
180	2.3477	2.2849	2.2303	2.1823	2.1397	2.1016	2.0672	2.0361	2.0077	1.9818
190	2.3425	2.2795	2.2249	2.1769	2.1343	2.0961	2.0618	2.0306	2.0023	1.9763
200	2.3375	2.2747	2.2201	2.1721	2.1294	2.0913	2.0569	2.0257	1.9973	1.9713
250	2.3193	2.2565	2.2018	2.1537	2.1110	2.0728	2.0384	2.0071	1.9786	1.9525
300	2.3073	2.2444	2.1897	2.1416	2.0988	2.0606	2.0261	1.9948	1.9662	1.9401
350	2.2987	2.2358	2.1811	2.1329	2.0901	2.0518	2.0173	1.9860	1.9574	1.9312
400	2.2923	2.2294	2.1746	2.1264	2.0836	2.0453	2.0107	1.9794	1.9508	1.9245
450	2.2873	2.2244	2.1696	2.1214	2.0786	2.0402	2.0057	1.9743	1.9456	1.9194
500	2.2833	2.2204	2.1656	2.1174	2.0746	2.0362	2.0016	1.9702	1.9415	1.9152
550	2.2800	2.2171	2.1624	2.1141	2.0713	2.0329	1.9983	1.9668	1.9382	1.9119
600	2.2773	2.2144	2.1596	2.1114	2.0685	2.0301	1.9955	1.9641	1.9354	1.9091
650	2.2750	2.2121	2.1573	2.1091	2.0662	2.0278	1.9932	1.9617	1.9330	1.9067

FISHER-QUANTILES EPS=0.050

FISHER-QUANTILES EPS=0.050

L/K	1	2	3	4	5	6	7	8	9	10
12	4.7472	3.8853	3.4903	3.2592	3.1059	2.9961	2.9134	2.8486	2.7964	2.7534
14	4.6001	3.7389	3.3439	3.1122	2.9582	2.8477	2.7642	2.6987	2.6458	2.6022
16	4.4940	3.6337	3.2389	3.0069	2.8524	2.7415	2.6572	2.5911	2.5377	2.4935
18	4.4139	3.5546	3.1599	2.9277	2.7729	2.6615	2.5767	2.5102	2.4563	2.4117
20	4.3512	3.4928	3.0984	2.8661	2.7109	2.5990	2.5140	2.4471	2.3928	2.3479
25	4.2417	3.3852	2.9912	2.7587	2.6030	2.4904	2.4047	2.3371	2.2821	2.2365
30	4.1709	3.3158	2.9223	2.6896	2.5336	2.4205	2.3343	2.2662	2.2107	2.1646
35	4.1215	3.2674	2.8742	2.6415	2.4851	2.3718	2.2852	2.2167	2.1608	2.1143
40	4.0847	3.2317	2.8387	2.6060	2.4495	2.3359	2.2490	2.1802	2.1240	2.0772
45	4.0566	3.2043	2.8115	2.5787	2.4221	2.3085	2.2212	2.1521	2.0958	2.0487
50	4.0343	3.1826	2.7900	2.5572	2.4004	2.2864	2.1992	2.1299	2.0734	2.0261
55	4.0167	3.1650	2.7725	2.5397	2.3828	2.2687	2.1813	2.1119	2.0552	2.0078
60	4.0012	3.1504	2.7581	2.5252	2.3683	2.2541	2.1665	2.0970	2.0401	1.9926
65	3.9886	3.1381	2.7459	2.5130	2.3560	2.2417	2.1541	2.0844	2.0274	1.9798
70	3.9778	3.1277	2.7355	2.5027	2.3456	2.2312	2.1435	2.0737	2.0166	1.9689
75	3.9685	3.1186	2.7266	2.4937	2.3366	2.2221	2.1343	2.0644	2.0073	1.9594
80	3.9604	3.1108	2.7188	2.4859	2.3287	2.2142	2.1263	2.0564	1.9991	1.9512
85	3.9532	3.1038	2.7119	2.4790	2.3218	2.2072	2.1193	2.0493	1.9919	1.9440
90	3.9469	3.0977	2.7058	2.4729	2.3157	2.2011	2.1131	2.0430	1.9856	1.9376
95	3.9412	3.0922	2.7004	2.4675	2.3102	2.1955	2.1075	2.0374	1.9799	1.9318
100	3.9361	3.0873	2.6955	2.4626	2.3053	2.1906	2.1025	2.0323	1.9748	1.9267
110	3.9274	3.0788	2.6871	2.4542	2.2969	2.1821	2.0939	2.0236	1.9661	1.9178
120	3.9201	3.0718	2.6802	2.4472	2.2899	2.1750	2.0868	2.0164	1.9588	1.9105
130	3.9140	3.0658	2.6743	2.4414	2.2839	2.1690	2.0807	2.0103	1.9526	1.9042
140	3.9087	3.0608	2.6693	2.4363	2.2789	2.1639	2.0756	2.0051	1.9473	1.8989
150	3.9042	3.0564	2.6649	2.4320	2.2745	2.1595	2.0711	2.0006	1.9428	1.8943
160	3.9002	3.0525	2.6611	2.4282	2.2707	2.1557	2.0672	1.9967	1.9388	1.8903
170	3.8967	3.0491	2.6578	2.4248	2.2673	2.1523	2.0638	1.9932	1.9353	1.8868
180	3.8936	3.0461	2.6548	2.4218	2.2643	2.1492	2.0608	1.9901	1.9322	1.8836
190	3.8909	3.0435	2.6521	2.4192	2.2616	2.1466	2.0580	1.9874	1.9294	1.8808
200	3.8884	3.0411	2.6498	2.4168	2.2592	2.1441	2.0556	1.9849	1.9269	1.8783
250	3.8789	3.0319	2.6407	2.4078	2.2501	2.1350	2.0463	1.9756	1.9174	1.8687
300	3.8726	3.0258	2.6347	2.4017	2.2441	2.1289	2.0402	1.9693	1.9112	1.8623
350	3.8682	3.0215	2.6304	2.3975	2.2398	2.1245	2.0358	1.9649	1.9067	1.8578
400	3.8648	3.0183	2.6272	2.3942	2.2366	2.1212	2.0325	1.9616	1.9033	1.8544
450	3.8622	3.0158	2.6247	2.3918	2.2340	2.1187	2.0299	1.9590	1.9007	1.8517
500	3.8601	3.0138	2.6227	2.3898	2.2320	2.1167	2.0279	1.9569	1.8986	1.8496
550	3.8584	3.0121	2.6211	2.3881	2.2304	2.1150	2.0262	1.9552	1.8969	1.8479
600	3.8570	3.0107	2.6198	2.3868	2.2290	2.1137	2.0248	1.9538	1.8955	1.8465
650	3.8558	3.0096	2.6186	2.3856	2.2279	2.1125	2.0237	1.9526	1.8943	1.8453

FISHER-QUANTILES EPS=0.050

L/K	11	12	13	14	15	16	17	18	19	20
12	2.7173									
14	2.5655	2.5542	2.5073							
16	2.4564	2.4247	2.3973	2.3755	2.3522					
18	2.3742	2.3421	2.3143	2.2900	2.2686	2.2496	2.2325			
20	2.3100	2.2776	2.2495	2.2250	2.2033	2.1840	2.1667	2.1511	2.1370	
25	2.1979	2.1649	2.1362	2.1111	2.0889	2.0691	2.0513	2.0355	2.0207	2.0075
30	2.1256	2.0921	2.0630	2.0374	2.0148	1.9946	1.9765	1.9601	1.9452	1.9317
35	2.0750	2.0411	2.0117	1.9858	1.9629	1.9424	1.9240	1.9075	1.8922	1.8784
40	2.0376	2.0035	1.9738	1.9476	1.9245	1.9037	1.8851	1.8682	1.8529	1.8389
45	2.0088	1.9745	1.9446	1.9182	1.8949	1.8740	1.8551	1.8381	1.8226	1.8084
50	1.9861	1.9515	1.9214	1.8949	1.8714	1.8503	1.8313	1.8141	1.7985	1.7841
55	1.9675	1.9329	1.9026	1.8760	1.8523	1.8311	1.8120	1.7946	1.7788	1.7644
60	1.9522	1.9174	1.8870	1.8602	1.8364	1.8151	1.7959	1.7784	1.7625	1.7480
65	1.9393	1.9044	1.8739	1.8470	1.8231	1.8017	1.7823	1.7648	1.7488	1.7342
70	1.9283	1.8932	1.8627	1.8357	1.8117	1.7902	1.7708	1.7531	1.7371	1.7223
75	1.9188	1.8836	1.8530	1.8259	1.8018	1.7802	1.7607	1.7430	1.7269	1.7121
80	1.9105	1.8753	1.8445	1.8174	1.7932	1.7716	1.7520	1.7342	1.7180	1.7032
85	1.9031	1.8679	1.8371	1.8099	1.7856	1.7639	1.7443	1.7265	1.7102	1.6953
90	1.8967	1.8613	1.8305	1.8032	1.7789	1.7571	1.7375	1.7196	1.7033	1.6883
95	1.8909	1.8555	1.8246	1.7973	1.7729	1.7511	1.7314	1.7134	1.6971	1.6821
100	1.8857	1.8503	1.8193	1.7919	1.7675	1.7456	1.7259	1.7079	1.6915	1.6764
110	1.8767	1.8412	1.8101	1.7827	1.7582	1.7363	1.7164	1.6984	1.6819	1.6667
120	1.8693	1.8337	1.8026	1.7750	1.7505	1.7285	1.7085	1.6904	1.6739	1.6587
130	1.8630	1.8273	1.7961	1.7686	1.7440	1.7219	1.7019	1.6837	1.6671	1.6519
140	1.8576	1.8219	1.7907	1.7630	1.7384	1.7162	1.6962	1.6780	1.6613	1.6460
150	1.8530	1.8172	1.7859	1.7582	1.7335	1.7113	1.6913	1.6730	1.6563	1.6410
160	1.8489	1.8131	1.7818	1.7540	1.7293	1.7071	1.6870	1.6687	1.6519	1.6366
170	1.8453	1.8095	1.7781	1.7504	1.7256	1.7033	1.6832	1.6648	1.6481	1.6327
180	1.8422	1.8063	1.7749	1.7471	1.7223	1.7000	1.6798	1.6614	1.6446	1.6292
190	1.8393	1.8034	1.7720	1.7441	1.7193	1.6970	1.6768	1.6584	1.6416	1.6261
200	1.8368	1.8008	1.7694	1.7415	1.7166	1.6943	1.6741	1.6556	1.6388	1.6233
250	1.8271	1.7910	1.7595	1.7315	1.7065	1.6841	1.6638	1.6453	1.6283	1.6127
300	1.8206	1.7845	1.7529	1.7249	1.6998	1.6773	1.6569	1.6383	1.6213	1.6057
350	1.8161	1.7799	1.7482	1.7201	1.6950	1.6725	1.6520	1.6334	1.6163	1.6006
400	1.8126	1.7764	1.7447	1.7166	1.6914	1.6688	1.6484	1.6297	1.6126	1.5969
450	1.8099	1.7737	1.7419	1.7138	1.6887	1.6660	1.6455	1.6268	1.6097	1.5939
500	1.8078	1.7715	1.7398	1.7116	1.6864	1.6638	1.6432	1.6245	1.6074	1.5916
550	1.8061	1.7698	1.7380	1.7098	1.6846	1.6619	1.6414	1.6226	1.6055	1.5897
600	1.8046	1.7683	1.7365	1.7083	1.6831	1.6604	1.6398	1.6211	1.6039	1.5881
650	1.8034	1.7671	1.7352	1.7070	1.6818	1.6591	1.6385	1.6197	1.6026	1.5867

FISHER-QUANTILES EPS=0.100

FISHER-QUANTILES EPS=0.100

L/K	1	2	3	4	5	6	7	8	9	10
12	3.1765	2.8568	2.6055	2.4801	2.3940	2.3310	2.2828	2.2446	2.2135	2.1878
14	3.1022	2.7865	2.5222	2.3947	2.3069	2.2426	2.1931	2.1539	2.1220	2.0954
16	3.0481	2.6682	2.4618	2.3327	2.2438	2.1785	2.1280	2.0880	2.0553	2.0281
18	3.0070	2.6239	2.4160	2.2858	2.1958	2.1296	2.0785	2.0379	2.0047	1.9776
20	2.9747	2.5893	2.3801	2.2489	2.1582	2.0915	2.0397	1.9985	1.9649	1.9367
25	2.9177	2.5283	2.3170	2.1842	2.0922	2.0241	1.9714	1.9292	1.8947	1.8656
30	2.8807	2.4887	2.2761	2.1422	2.0492	1.9803	1.9269	1.8841	1.8490	1.8195
35	2.8547	2.4609	2.2474	2.1128	2.0191	1.9496	1.8957	1.8524	1.8168	1.7859
40	2.8354	2.4404	2.2261	2.0909	1.9968	1.9269	1.8725	1.8289	1.7929	1.7627
45	2.8205	2.4245	2.2097	2.0742	1.9796	1.9094	1.8547	1.8107	1.7745	1.7440
50	2.8087	2.4119	2.1967	2.0608	1.9660	1.8954	1.8405	1.7965	1.7596	1.7291
55	2.7990	2.4017	2.1862	2.0500	1.9549	1.8841	1.8290	1.7846	1.7479	1.7171
60	2.7911	2.3933	2.1774	2.0410	1.9457	1.8747	1.8194	1.7748	1.7380	1.7070
65	2.7843	2.3861	2.1700	2.0334	1.9380	1.8668	1.8113	1.7666	1.7297	1.6985
70	2.7786	2.3800	2.1637	2.0269	1.9313	1.8600	1.8044	1.7596	1.7225	1.6913
75	2.7736	2.3747	2.1583	2.0214	1.9256	1.8542	1.7985	1.7535	1.7164	1.6850
80	2.7693	2.3701	2.1535	2.0165	1.9206	1.8491	1.7933	1.7483	1.7110	1.6796
85	2.7655	2.3661	2.1494	2.0122	1.9162	1.8446	1.7887	1.7436	1.7063	1.6748
90	2.7621	2.3625	2.1457	2.0084	1.9123	1.8406	1.7846	1.7395	1.7021	1.6705
95	2.7591	2.3593	2.1424	2.0050	1.9089	1.8371	1.7810	1.7358	1.6983	1.6667
100	2.7564	2.3564	2.1394	2.0019	1.9057	1.8339	1.7778	1.7324	1.6949	1.6632
110	2.7517	2.3515	2.1343	1.9967	1.9004	1.8284	1.7721	1.7267	1.6891	1.6573
120	2.7478	2.3473	2.1300	1.9923	1.8959	1.8238	1.7675	1.7220	1.6842	1.6524
130	2.7445	2.3439	2.1264	1.9886	1.8921	1.8199	1.7635	1.7179	1.6802	1.6482
140	2.7417	2.3409	2.1233	1.9854	1.8889	1.8166	1.7602	1.7145	1.6767	1.6447
150	2.7393	2.3383	2.1207	1.9827	1.8861	1.8138	1.7572	1.7115	1.6736	1.6416
160	2.7371	2.3360	2.1183	1.9803	1.8836	1.8113	1.7547	1.7089	1.6710	1.6389
170	2.7353	2.3341	2.1163	1.9782	1.8815	1.8091	1.7524	1.7066	1.6686	1.6365
180	2.7336	2.3323	2.1145	1.9764	1.8795	1.8071	1.7504	1.7046	1.6666	1.6344
190	2.7321	2.3307	2.1128	1.9747	1.8778	1.8054	1.7486	1.7028	1.6647	1.6325
200	2.7308	2.3293	2.1114	1.9732	1.8763	1.8038	1.7470	1.7011	1.6630	1.6308
250	2.7257	2.3239	2.1058	1.9675	1.8704	1.7978	1.7409	1.6949	1.6567	1.6244
300	2.7225	2.3203	2.1021	1.9637	1.8666	1.7938	1.7369	1.6908	1.6525	1.6201
350	2.7199	2.3178	2.0995	1.9610	1.8638	1.7910	1.7340	1.6878	1.6495	1.6170
400	2.7181	2.3159	2.0975	1.9590	1.8617	1.7889	1.7318	1.6856	1.6472	1.6147
450	2.7167	2.3144	2.0960	1.9574	1.8601	1.7872	1.7301	1.6839	1.6455	1.6129
500	2.7156	2.3132	2.0948	1.9561	1.8588	1.7859	1.7288	1.6825	1.6441	1.6115
550	2.7147	2.3123	2.0938	1.9551	1.8578	1.7849	1.7277	1.6814	1.6429	1.6103
600	2.7139	2.3114	2.0929	1.9543	1.8569	1.7840	1.7268	1.6805	1.6420	1.6094
650	2.7133	2.3108	2.0922	1.9535	1.8562	1.7832	1.7260	1.6797	1.6412	1.6086

FISHER-QUANTILES EPS=0.100

L/K	11	12	13	14	15	16	17	18	19	20
12	2.1660									
14	2.0729	2.0557	2.0370							
16	2.0051	1.9854	1.9682	1.9532	1.9399					
18	1.9535	1.9353	1.9158	1.9004	1.8868	1.8747	1.8638			
20	1.9129	1.8924	1.8745	1.8588	1.8449	1.8325	1.8214	1.8113	1.8022	
25	1.8412	1.8200	1.8015	1.7853	1.7708	1.7579	1.7463	1.7358	1.7263	1.7175
30	1.7944	1.7727	1.7538	1.7371	1.7223	1.7090	1.6970	1.6862	1.6763	1.6673
35	1.7614	1.7394	1.7201	1.7031	1.6880	1.6744	1.6622	1.6511	1.6410	1.6317
40	1.7369	1.7146	1.6950	1.6778	1.6624	1.6486	1.6362	1.6249	1.6146	1.6052
45	1.7180	1.6954	1.6757	1.6582	1.6426	1.6287	1.6161	1.6046	1.5941	1.5846
50	1.7029	1.6802	1.6602	1.6426	1.6269	1.6128	1.6000	1.5884	1.5778	1.5681
55	1.6906	1.6677	1.6477	1.6299	1.6140	1.5998	1.5869	1.5752	1.5645	1.5547
60	1.6805	1.6574	1.6372	1.6193	1.6034	1.5890	1.5760	1.5642	1.5534	1.5435
65	1.6719	1.6487	1.6284	1.6104	1.5943	1.5799	1.5668	1.5549	1.5440	1.5340
70	1.6645	1.6413	1.6209	1.6028	1.5866	1.5721	1.5589	1.5470	1.5360	1.5259
75	1.6582	1.6348	1.6143	1.5962	1.5799	1.5653	1.5521	1.5401	1.5290	1.5189
80	1.6526	1.6292	1.6086	1.5904	1.5741	1.5594	1.5461	1.5340	1.5230	1.5128
85	1.6477	1.6243	1.6036	1.5853	1.5690	1.5542	1.5409	1.5287	1.5176	1.5073
90	1.6434	1.6199	1.5992	1.5808	1.5644	1.5496	1.5362	1.5240	1.5128	1.5025
95	1.6395	1.6159	1.5952	1.5768	1.5603	1.5455	1.5320	1.5198	1.5085	1.4982
100	1.6360	1.6124	1.5916	1.5731	1.5566	1.5418	1.5283	1.5160	1.5047	1.4943
110	1.6300	1.6063	1.5854	1.5669	1.5503	1.5355	1.5218	1.5094	1.4981	1.4877
120	1.6250	1.6012	1.5803	1.5617	1.5450	1.5300	1.5164	1.5039	1.4926	1.4821
130	1.6208	1.5969	1.5759	1.5572	1.5405	1.5255	1.5118	1.4993	1.4879	1.4773
140	1.6172	1.5932	1.5722	1.5535	1.5367	1.5216	1.5079	1.4954	1.4839	1.4733
150	1.6140	1.5901	1.5690	1.5502	1.5334	1.5182	1.5045	1.4919	1.4804	1.4698
160	1.6113	1.5873	1.5661	1.5473	1.5305	1.5153	1.5015	1.4889	1.4774	1.4667
170	1.6089	1.5848	1.5636	1.5448	1.5279	1.5127	1.4989	1.4863	1.4747	1.4640
180	1.6067	1.5826	1.5614	1.5426	1.5257	1.5104	1.4966	1.4839	1.4723	1.4616
190	1.6048	1.5807	1.5595	1.5406	1.5236	1.5084	1.4945	1.4818	1.4702	1.4595
200	1.6031	1.5789	1.5577	1.5388	1.5218	1.5065	1.4926	1.4799	1.4683	1.4575
250	1.5965	1.5723	1.5509	1.5319	1.5149	1.4995	1.4855	1.4727	1.4610	1.4501
300	1.5922	1.5679	1.5464	1.5273	1.5102	1.4948	1.4807	1.4679	1.4561	1.4452
350	1.5891	1.5647	1.5432	1.5241	1.5069	1.4914	1.4773	1.4645	1.4526	1.4417
400	1.5867	1.5623	1.5408	1.5216	1.5045	1.4889	1.4748	1.4619	1.4500	1.4391
450	1.5849	1.5605	1.5389	1.5198	1.5025	1.4870	1.4728	1.4599	1.4480	1.4370
500	1.5835	1.5590	1.5374	1.5182	1.5010	1.4854	1.4712	1.4583	1.4464	1.4354
550	1.5823	1.5578	1.5362	1.5170	1.4997	1.4841	1.4699	1.4570	1.4450	1.4340
600	1.5813	1.5568	1.5352	1.5160	1.4987	1.4831	1.4689	1.4559	1.4439	1.4329
650	1.5805	1.5560	1.5343	1.5151	1.4978	1.4822	1.4680	1.4549	1.4430	1.4320

FISHER-QUANTILES EPS=0.200

FISHER-QUANTILES

EPS=0.200

L/K	1	2	3	4	5	6	7	8	9	10
12	1.8393	1.8466	1.8042	1.7684	1.7403	1.7182	1.7003	1.6856	1.6734	1.6630
14	1.8091	1.8095	1.7646	1.7287	1.6971	1.6736	1.6547	1.6392	1.6262	1.6152
16	1.7869	1.7828	1.7355	1.6961	1.6653	1.6409	1.6212	1.6050	1.5915	1.5800
18	1.7699	1.7623	1.7134	1.6727	1.6410	1.6159	1.5956	1.5788	1.5648	1.5528
20	1.7565	1.7462	1.6958	1.6543	1.6218	1.5960	1.5752	1.5581	1.5436	1.5313
25	1.7328	1.7176	1.6648	1.6215	1.5877	1.5609	1.5391	1.5211	1.5060	1.4931
30	1.7172	1.6990	1.6445	1.6001	1.5654	1.5378	1.5154	1.4968	1.4812	1.4678
35	1.7062	1.6858	1.6302	1.5850	1.5496	1.5215	1.4986	1.4796	1.4636	1.4499
40	1.6980	1.6760	1.6195	1.5737	1.5379	1.5093	1.4861	1.4668	1.4505	1.4365
45	1.6917	1.6684	1.6113	1.5650	1.5288	1.4999	1.4764	1.4569	1.4404	1.4262
50	1.6867	1.6624	1.6048	1.5581	1.5216	1.4924	1.4687	1.4490	1.4323	1.4179
55	1.6826	1.6575	1.5994	1.5524	1.5157	1.4863	1.4624	1.4425	1.4256	1.4111
60	1.6792	1.6534	1.5950	1.5478	1.5108	1.4813	1.4572	1.4371	1.4201	1.4055
65	1.6763	1.6500	1.5913	1.5438	1.5066	1.4770	1.4528	1.4326	1.4155	1.4008
70	1.6738	1.6470	1.5881	1.5404	1.5031	1.4733	1.4490	1.4287	1.4115	1.3967
75	1.6717	1.6445	1.5853	1.5375	1.5001	1.4702	1.4457	1.4254	1.4081	1.3932
80	1.6698	1.6423	1.5829	1.5349	1.4974	1.4674	1.4429	1.4224	1.4051	1.3901
85	1.6682	1.6403	1.5808	1.5327	1.4950	1.4650	1.4404	1.4198	1.4024	1.3874
90	1.6668	1.6386	1.5789	1.5307	1.4930	1.4628	1.4381	1.4175	1.4001	1.3850
95	1.6655	1.6370	1.5772	1.5289	1.4911	1.4609	1.4361	1.4155	1.3980	1.3828
100	1.6643	1.6356	1.5757	1.5273	1.4894	1.4591	1.4343	1.4136	1.3961	1.3809
110	1.6623	1.6332	1.5731	1.5245	1.4865	1.4561	1.4312	1.4105	1.3928	1.3775
120	1.6606	1.6312	1.5709	1.5222	1.4841	1.4536	1.4287	1.4078	1.3901	1.3748
130	1.6592	1.6295	1.5691	1.5203	1.4821	1.4515	1.4265	1.4056	1.3878	1.3724
140	1.6580	1.6281	1.5675	1.5186	1.4803	1.4497	1.4246	1.4036	1.3858	1.3704
150	1.6569	1.6268	1.5661	1.5172	1.4788	1.4481	1.4230	1.4020	1.3841	1.3686
160	1.6560	1.6257	1.5649	1.5159	1.4775	1.4468	1.4216	1.4005	1.3826	1.3671
170	1.6552	1.6248	1.5639	1.5148	1.4763	1.4456	1.4203	1.3992	1.3813	1.3658
180	1.6545	1.6239	1.5630	1.5138	1.4753	1.4445	1.4192	1.3981	1.3801	1.3646
190	1.6539	1.6231	1.5621	1.5130	1.4744	1.4435	1.4182	1.3971	1.3790	1.3635
200	1.6533	1.6225	1.5614	1.5122	1.4736	1.4427	1.4173	1.3962	1.3781	1.3625
250	1.6511	1.6198	1.5585	1.5091	1.4704	1.4394	1.4140	1.3927	1.3745	1.3586
300	1.6496	1.6181	1.5566	1.5071	1.4683	1.4372	1.4117	1.3903	1.3721	1.3564
350	1.6486	1.6169	1.5553	1.5057	1.4668	1.4357	1.4101	1.3887	1.3704	1.3547
400	1.6478	1.6159	1.5543	1.5046	1.4657	1.4345	1.4089	1.3874	1.3692	1.3533
450	1.6472	1.6152	1.5535	1.5038	1.4648	1.4336	1.4080	1.3865	1.3682	1.3523
500	1.6467	1.6146	1.5529	1.5031	1.4641	1.4329	1.4072	1.3857	1.3674	1.3515
550	1.6463	1.6142	1.5523	1.5026	1.4635	1.4323	1.4066	1.3851	1.3667	1.3508
600	1.6460	1.6138	1.5519	1.5021	1.4631	1.4318	1.4061	1.3845	1.3662	1.3503
650	1.6457	1.6134	1.5516	1.5018	1.4627	1.4314	1.4056	1.3841	1.3657	1.3498

PHI-QUANTILES EPS=0.010

L/K	11	12	13	14	15	16	17	18	19	20
12	3.5158									
14	3.1691	3.1565	3.1456							
16	2.9262	2.9158	2.9068	2.8990	2.8834					
18	2.7464	2.7369	2.7287	2.7211	2.7022	2.6944	2.6874			
20	2.6079	2.5990	2.5920	2.5776	2.5625	2.5544	2.5472	2.5407	2.5349	
25	2.3694	2.3548	2.3421	2.3311	2.3214	2.3129	2.3052	2.2984	2.2922	2.2865
30	2.2172	2.2020	2.1888	2.1774	2.1673	2.1585	2.1503	2.1431	2.1366	2.1308
35	2.1114	2.0956	2.0821	2.0702	2.0598	2.0505	2.0422	2.0347	2.0280	2.0218
40	2.0332	2.0172	2.0034	1.9916	1.9804	1.9708	1.9623	1.9546	1.9476	1.9413
45	1.9732	1.9569	1.9426	1.9302	1.9193	1.9099	1.9007	1.8928	1.8856	1.8791
50	1.9255	1.9089	1.8945	1.8820	1.8705	1.8606	1.8518	1.8441	1.8376	1.8296
55	1.8867	1.8698	1.8551	1.8423	1.8310	1.8211	1.8116	1.8034	1.7961	1.7897
60	1.8545	1.8374	1.8225	1.8094	1.7979	1.7876	1.7785	1.7706	1.7623	1.7555
65	1.8274	1.8100	1.7949	1.7817	1.7700	1.7595	1.7502	1.7418	1.7344	1.7280
70	1.8041	1.7866	1.7713	1.7579	1.7461	1.7355	1.7260	1.7174	1.7096	1.7027
75	1.7840	1.7663	1.7509	1.7374	1.7254	1.7146	1.7050	1.6963	1.6884	1.6812
80	1.7664	1.7485	1.7330	1.7194	1.7072	1.6964	1.6867	1.6778	1.6698	1.6625
85	1.7508	1.7329	1.7172	1.7035	1.6912	1.6803	1.6704	1.6615	1.6534	1.6460
90	1.7370	1.7190	1.7032	1.6893	1.6770	1.6660	1.6561	1.6470	1.6388	1.6314
95	1.7247	1.7065	1.6906	1.6766	1.6642	1.6531	1.6431	1.6341	1.6258	1.6182
100	1.7142	1.6953	1.6793	1.6652	1.6527	1.6415	1.6314	1.6223	1.6141	1.6063
110	1.6946	1.6766	1.6614	1.6435	1.6328	1.6215	1.6112	1.6020	1.5936	1.5859
120	1.6784	1.6609	1.6442	1.6308	1.6162	1.6047	1.5944	1.5850	1.5764	1.5686
130	1.6648	1.6461	1.6289	1.6150	1.6042	1.5946	1.5800	1.5706	1.5619	1.5540
140	1.6531	1.6343	1.6178	1.6035	1.5911	1.5807	1.5722	1.5581	1.5494	1.5414
150	1.6430	1.6240	1.6074	1.5929	1.5801	1.5691	1.5598	1.5524	1.5472	1.5304
160	1.6342	1.6150	1.5983	1.5836	1.5706	1.5592	1.5494	1.5411	1.5347	1.5504
170	1.6263	1.6071	1.5903	1.5754	1.5623	1.5506	1.5404	1.5310	1.5244	1.5189
180	1.6194	1.6001	1.5831	1.5682	1.5549	1.5431	1.5326	1.5234	1.5156	1.5093
190	1.6131	1.5937	1.5767	1.5617	1.5483	1.5364	1.5257	1.5163	1.5081	1.5011
200	1.6075	1.5881	1.5710	1.5559	1.5424	1.5304	1.5196	1.5099	1.5014	1.4941
250	1.5861	1.5664	1.5490	1.5337	1.5199	1.5076	1.4964	1.4865	1.4771	1.4687
300	1.5718	1.5518	1.5343	1.5188	1.5048	1.4923	1.4810	1.4706	1.4612	1.4525
350	1.5615	1.5414	1.5238	1.5081	1.4940	1.4814	1.4699	1.4594	1.4499	1.4411
400	1.5538	1.5336	1.5158	1.5000	1.4859	1.4731	1.4615	1.4510	1.4413	1.4324
450	1.5478	1.5275	1.5096	1.4937	1.4795	1.4667	1.4550	1.4444	1.4347	1.4257
500	1.5430	1.5226	1.5046	1.4887	1.4744	1.4615	1.4498	1.4391	1.4293	1.4203
550	1.5390	1.5185	1.5005	1.4845	1.4702	1.4572	1.4455	1.4348	1.4249	1.4158
600	1.5356	1.5152	1.4971	1.4811	1.4667	1.4537	1.4419	1.4311	1.4212	1.4121
650	1.5327	1.5122	1.4942	1.4781	1.4637	1.4507	1.4388	1.4280	1.4181	1.4089

PHI-QUANTILES EPS=0.050

L/K	1	2	3	4	5	6	7	8	9	10
12	2.7003	2.5628	2.4954	2.4553	2.4287	2.4097	2.3955	2.3845	2.3757	2.3685
14	2.5702	2.4276	2.3534	2.3092	2.2798	2.2587	2.2429	2.2306	2.2207	2.2126
16	2.4920	2.3303	2.2511	2.2038	2.1722	2.1495	2.1324	2.1190	2.1083	2.0995
18	2.4264	2.2569	2.1739	2.1241	2.0907	2.0667	2.0486	2.0344	2.0230	2.0136
20	2.3751	2.1995	2.1134	2.0616	2.0268	2.0018	1.9828	1.9679	1.9559	1.9460
25	2.2856	2.0992	2.0075	1.9520	1.9145	1.8874	1.8667	1.8505	1.8374	1.8265
30	2.2278	2.0343	1.9389	1.8808	1.8414	1.8127	1.7908	1.7736	1.7596	1.7480
35	2.1874	1.9869	1.8907	1.8307	1.7898	1.7600	1.7372	1.7191	1.7045	1.6923
40	2.1576	1.9553	1.8580	1.7965	1.7545	1.7208	1.6972	1.6785	1.6633	1.6506
45	2.1347	1.9295	1.8274	1.7648	1.7219	1.6904	1.6662	1.6470	1.6313	1.6183
50	2.1165	1.9090	1.8056	1.7420	1.6983	1.6662	1.6415	1.6218	1.6057	1.5924
55	2.1018	1.8923	1.7878	1.7234	1.6790	1.6464	1.6213	1.6012	1.5848	1.5711
60	2.0896	1.8785	1.7730	1.7079	1.6630	1.6300	1.6044	1.5840	1.5673	1.5534
65	2.0795	1.8669	1.7606	1.6949	1.6495	1.6160	1.5902	1.5695	1.5525	1.5384
70	2.0706	1.8569	1.7499	1.6837	1.6379	1.6041	1.5780	1.5570	1.5399	1.5255
75	2.0630	1.8484	1.7407	1.6741	1.6279	1.5938	1.5674	1.5462	1.5288	1.5143
80	2.0564	1.8409	1.7327	1.6656	1.6192	1.5848	1.5581	1.5367	1.5192	1.5045
85	2.0506	1.8343	1.7256	1.6582	1.6114	1.5768	1.5499	1.5284	1.5106	1.4958
90	2.0455	1.8284	1.7194	1.6516	1.6046	1.5697	1.5426	1.5209	1.5030	1.4880
95	2.0409	1.8232	1.7138	1.6457	1.5984	1.5634	1.5361	1.5142	1.4962	1.4811
100	2.0367	1.8185	1.7087	1.6404	1.5929	1.5577	1.5303	1.5082	1.4901	1.4748
110	2.0296	1.8104	1.7000	1.6312	1.5834	1.5478	1.5201	1.4978	1.4795	1.4640
120	2.0237	1.8037	1.6928	1.6236	1.5754	1.5396	1.5116	1.4892	1.4706	1.4550
130	2.0187	1.7980	1.6867	1.6172	1.5687	1.5326	1.5045	1.4818	1.4631	1.4473
140	2.0145	1.7932	1.6815	1.6116	1.5630	1.5267	1.4983	1.4755	1.4566	1.4407
150	2.0107	1.7890	1.6769	1.6069	1.5580	1.5215	1.4930	1.4700	1.4510	1.4350
160	2.0075	1.7853	1.6730	1.6027	1.5536	1.5169	1.4883	1.4652	1.4461	1.4299
170	2.0045	1.7821	1.6695	1.5990	1.5497	1.5129	1.4842	1.4610	1.4417	1.4255
180	2.0018	1.7792	1.6664	1.5957	1.5463	1.5094	1.4805	1.4572	1.4379	1.4215
190	1.9993	1.7766	1.6636	1.5928	1.5432	1.5062	1.4772	1.4538	1.4344	1.4180
200	1.9970	1.7743	1.6611	1.5901	1.5405	1.5035	1.4743	1.4508	1.4313	1.4148
250	1.9861	1.7631	1.6515	1.5801	1.5300	1.4924	1.4630	1.4392	1.4194	1.4026
300	1.9745	1.7580	1.6448	1.5733	1.5229	1.4851	1.4555	1.4314	1.4114	1.3944
350	1.9611	1.7514	1.6394	1.5681	1.5177	1.4798	1.4500	1.4256	1.4057	1.3886
400	1.9457	1.7445	1.6345	1.5637	1.5135	1.4757	1.4458	1.4215	1.4013	1.3841
450	1.9285	1.7371	1.6295	1.5596	1.5099	1.4721	1.4424	1.4181	1.3978	1.3806
500	1.9097	1.7290	1.6243	1.5556	1.5064	1.4690	1.4393	1.4151	1.3949	1.3777
550	1.8895	1.7203	1.6188	1.5515	1.5030	1.4659	1.4365	1.4124	1.3923	1.3751
600	1.8684	1.7111	1.6130	1.5472	1.4995	1.4629	1.4338	1.4099	1.3899	1.3728
650	1.8463	1.7013	1.6068	1.5427	1.4959	1.4599	1.4311	1.4075	1.3876	1.3706

PHI-QUANTILES EPS=0.050

L/K	11	12	13	14	15	16	17	18	19	20
12	2.3624									
14	2.2058	2.2001	2.1952							
16	2.0922	2.0860	2.0806	2.0760	2.0719					
18	2.0058	1.9991	1.9934	1.9884	1.9841	1.9802	1.9767			
20	1.9378	1.9307	1.9247	1.9194	1.9148	1.9107	1.9071	1.9038	1.9008	
25	1.8174	1.8096	1.8029	1.7971	1.7919	1.7874	1.7833	1.7797	1.7764	1.7734
30	1.7582	1.7500	1.7427	1.7364	1.7309	1.7260	1.7216	1.7176	1.7140	1.7108
35	1.6821	1.6733	1.6657	1.6590	1.6531	1.6479	1.6432	1.6390	1.6352	1.6318
40	1.6600	1.6508	1.6429	1.6359	1.6298	1.6243	1.6195	1.6150	1.6110	1.6074
45	1.6072	1.5978	1.5895	1.5823	1.5760	1.5703	1.5652	1.5606	1.5565	1.5530
50	1.5810	1.5713	1.5628	1.5554	1.5488	1.5429	1.5377	1.5329	1.5286	1.5247
55	1.5595	1.5495	1.5408	1.5332	1.5265	1.5204	1.5150	1.5102	1.5058	1.5020
60	1.5416	1.5314	1.5225	1.5147	1.5078	1.5016	1.4961	1.4910	1.4865	1.4824
65	1.5263	1.5159	1.5069	1.4990	1.4919	1.4856	1.4799	1.4748	1.4701	1.4659
70	1.5132	1.5027	1.4935	1.4854	1.4782	1.4718	1.4660	1.4608	1.4560	1.4517
75	1.5019	1.4912	1.4818	1.4736	1.4663	1.4598	1.4539	1.4486	1.4438	1.4393
80	1.4919	1.4811	1.4716	1.4633	1.4559	1.4493	1.4433	1.4379	1.4330	1.4285
85	1.4832	1.4721	1.4626	1.4541	1.4466	1.4399	1.4339	1.4284	1.4234	1.4188
90	1.4753	1.4643	1.4545	1.4459	1.4384	1.4316	1.4254	1.4199	1.4148	1.4102
95	1.4682	1.4571	1.4475	1.4386	1.4309	1.4241	1.4179	1.4122	1.4071	1.4024
100	1.4618	1.4506	1.4409	1.4320	1.4242	1.4173	1.4110	1.4054	1.4002	1.3954
110	1.4508	1.4394	1.4294	1.4207	1.4131	1.4056	1.3992	1.3934	1.3881	1.3832
120	1.4416	1.4300	1.4199	1.4110	1.4031	1.3962	1.3904	1.3835	1.3779	1.3730
130	1.4338	1.4221	1.4118	1.4027	1.3947	1.3876	1.3813	1.3760	1.3693	1.3643
140	1.4271	1.4152	1.4049	1.3957	1.3875	1.3802	1.3737	1.3681	1.3632	1.3595
150	1.4212	1.4093	1.3988	1.3895	1.3813	1.3739	1.3672	1.3615	1.3562	1.3516
160	1.4161	1.4041	1.3935	1.3842	1.3758	1.3683	1.3616	1.3555	1.3501	1.3454
170	1.4116	1.3995	1.3888	1.3794	1.3710	1.3634	1.3566	1.3504	1.3449	1.3399
180	1.4075	1.3953	1.3846	1.3752	1.3667	1.3590	1.3521	1.3459	1.3402	1.3351
190	1.4039	1.3917	1.3809	1.3713	1.3628	1.3551	1.3482	1.3418	1.3361	1.3309
200	1.4006	1.3883	1.3775	1.3679	1.3593	1.3516	1.3446	1.3382	1.3324	1.3271
250	1.3882	1.3756	1.3646	1.3548	1.3460	1.3380	1.3309	1.3245	1.3183	1.3128
300	1.3799	1.3671	1.3559	1.3459	1.3370	1.3289	1.3216	1.3149	1.3088	1.3031
350	1.3739	1.3610	1.3497	1.3396	1.3305	1.3224	1.3149	1.3082	1.3019	1.2962
400	1.3693	1.3564	1.3450	1.3348	1.3257	1.3174	1.3099	1.3031	1.2968	1.2910
450	1.3657	1.3527	1.3413	1.3310	1.3218	1.3135	1.3060	1.2991	1.2927	1.2869
500	1.3628	1.3497	1.3382	1.3280	1.3187	1.3104	1.3028	1.2958	1.2894	1.2836
550	1.3602	1.3472	1.3357	1.3254	1.3161	1.3078	1.3001	1.2932	1.2867	1.2808
600	1.3579	1.3450	1.3334	1.3232	1.3139	1.3055	1.2979	1.2909	1.2844	1.2785
650	1.3558	1.3429	1.3314	1.3212	1.3119	1.3035	1.2959	1.2889	1.2824	1.2765

PHI-QUANTILES EPS=0.100

I/K	1	2	3	4	5	6	7	8	9	10
12	2.0712	2.0233	2.0000	1.9818	1.9603	1.9602	1.9533	1.9479	1.9435	1.9400
14	2.0132	1.9479	1.9136	1.8918	1.8768	1.8659	1.8574	1.8511	1.8458	1.8415
16	1.9558	1.8894	1.8506	1.8260	1.8090	1.7967	1.7873	1.7799	1.7739	1.7690
18	1.9164	1.8449	1.8026	1.7757	1.7572	1.7437	1.7334	1.7253	1.7187	1.7133
20	1.8870	1.8090	1.7647	1.7366	1.7162	1.7017	1.6907	1.6819	1.6749	1.6690
25	1.8354	1.7433	1.6978	1.6657	1.6435	1.6271	1.6145	1.6046	1.5965	1.5898
30	1.8019	1.7031	1.6521	1.6196	1.5955	1.5778	1.5642	1.5533	1.5445	1.5371
35	1.7784	1.6793	1.6282	1.5969	1.5736	1.5428	1.5283	1.5167	1.5073	1.4996
40	1.7610	1.6581	1.6002	1.5625	1.5382	1.5166	1.5014	1.4893	1.4793	1.4711
45	1.7476	1.6427	1.5825	1.5437	1.5185	1.4962	1.4805	1.4679	1.4575	1.4489
50	1.7370	1.6293	1.5683	1.5286	1.5007	1.4799	1.4637	1.4507	1.4400	1.4311
55	1.7284	1.6194	1.5568	1.5164	1.4879	1.4666	1.4500	1.4366	1.4257	1.4165
60	1.7212	1.6107	1.5472	1.5062	1.4771	1.4554	1.4385	1.4249	1.4137	1.4042
65	1.7152	1.6034	1.5392	1.4975	1.4681	1.4460	1.4288	1.4149	1.4035	1.3938
70	1.7100	1.5971	1.5322	1.4901	1.4603	1.4379	1.4206	1.4063	1.3947	1.3849
75	1.7056	1.5917	1.5262	1.4837	1.4536	1.4309	1.4132	1.3989	1.3871	1.3771
80	1.7017	1.5871	1.5210	1.4781	1.4477	1.4248	1.4069	1.3924	1.3804	1.3703
85	1.6983	1.5828	1.5164	1.4732	1.4426	1.4194	1.4013	1.3866	1.3745	1.3643
90	1.6953	1.5791	1.5123	1.4688	1.4379	1.4146	1.3963	1.3815	1.3692	1.3589
95	1.6926	1.5758	1.5087	1.4649	1.4337	1.4103	1.3918	1.3769	1.3645	1.3540
100	1.6901	1.5729	1.5054	1.4614	1.4300	1.4064	1.3878	1.3727	1.3602	1.3497
110	1.6859	1.5678	1.4997	1.4553	1.4236	1.3997	1.3808	1.3655	1.3529	1.3421
120	1.6824	1.5635	1.4950	1.4502	1.4182	1.3941	1.3750	1.3595	1.3467	1.3358
130	1.6793	1.5599	1.4910	1.4459	1.4137	1.3893	1.3701	1.3544	1.3415	1.3305
140	1.6766	1.5569	1.4876	1.4423	1.4098	1.3852	1.3658	1.3501	1.3370	1.3258
150	1.6740	1.5543	1.4847	1.4391	1.4064	1.3817	1.3622	1.3463	1.3331	1.3218
160	1.6716	1.5519	1.4821	1.4363	1.4035	1.3786	1.3590	1.3430	1.3296	1.3183
170	1.6693	1.5498	1.4798	1.4338	1.4009	1.3759	1.3561	1.3400	1.3266	1.3152
180	1.6672	1.5479	1.4778	1.4316	1.3986	1.3735	1.3536	1.3374	1.3239	1.3124
190	1.6652	1.5461	1.4759	1.4297	1.3965	1.3713	1.3513	1.3351	1.3215	1.3100
200	1.6615	1.5445	1.4743	1.4279	1.3946	1.3693	1.3493	1.3330	1.3193	1.3077
250	1.6454	1.5371	1.4676	1.4211	1.3875	1.3619	1.3415	1.3249	1.3110	1.2992
300	1.6339	1.5292	1.4620	1.4160	1.3825	1.3568	1.3363	1.3195	1.3054	1.2934
350	1.5973	1.5190	1.4567	1.4115	1.3786	1.3528	1.3323	1.3155	1.3013	1.2893
400	1.5662	1.5089	1.4500	1.4069	1.3744	1.3493	1.3290	1.3122	1.2981	1.2860
450	1.5511	1.4969	1.4438	1.4019	1.3706	1.3460	1.3260	1.3094	1.2954	1.2833
500	1.4922	1.4821	1.4347	1.3964	1.3664	1.3425	1.3230	1.3066	1.2928	1.2809
550	1.4498	1.4667	1.4258	1.3903	1.3619	1.3388	1.3198	1.3039	1.2903	1.2785
600	1.4136	1.4501	1.4162	1.3838	1.3569	1.3349	1.3165	1.3010	1.2877	1.2762
650	1.3529	1.4326	1.4060	1.3787	1.3536	1.3307	1.3130	1.2980	1.2851	1.2738

PHI-QUANTILES EPS=0.100

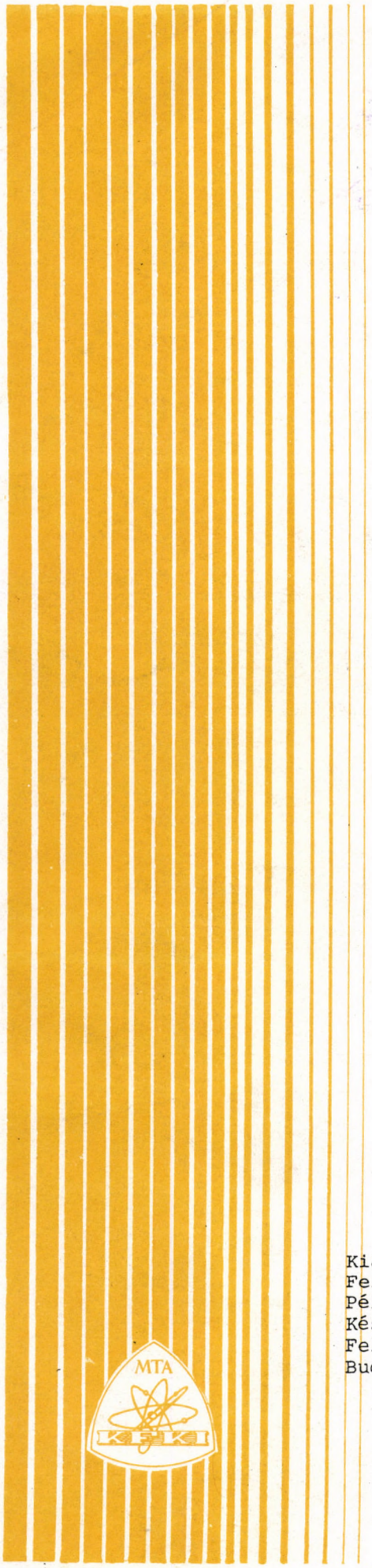
L/K	11	12	13	14	15	16	17	18	19	20
12	1.9370									
14	1.8379	1.8348	1.8322							
16	1.7649	1.7614	1.7584	1.7558	1.7535					
18	1.7088	1.7049	1.7016	1.6987	1.6961	1.6939	1.6918			
20	1.6641	1.6599	1.6563	1.6532	1.6504	1.6480	1.6458	1.6438	1.6421	
25	1.5842	1.5794	1.5752	1.5716	1.5684	1.5655	1.5630	1.5607	1.5586	1.5567
30	1.5309	1.5256	1.5210	1.5170	1.5135	1.5103	1.5075	1.5049	1.5026	1.5006
35	1.4928	1.4871	1.4821	1.4778	1.4740	1.4706	1.4675	1.4648	1.4623	1.4600
40	1.4640	1.4580	1.4528	1.4482	1.4442	1.4405	1.4373	1.4344	1.4318	1.4293
45	1.4416	1.4353	1.4298	1.4250	1.4207	1.4169	1.4136	1.4104	1.4076	1.4051
50	1.4235	1.4170	1.4113	1.4063	1.4018	1.3979	1.3943	1.3911	1.3883	1.3855
55	1.4087	1.4019	1.3960	1.3909	1.3863	1.3822	1.3785	1.3752	1.3721	1.3694
60	1.3962	1.3893	1.3833	1.3779	1.3732	1.3690	1.3652	1.3617	1.3586	1.3558
65	1.3856	1.3786	1.3724	1.3669	1.3621	1.3577	1.3538	1.3503	1.3471	1.3442
70	1.3765	1.3693	1.3630	1.3574	1.3525	1.3480	1.3440	1.3404	1.3371	1.3341
75	1.3686	1.3613	1.3548	1.3492	1.3441	1.3396	1.3355	1.3318	1.3284	1.3254
80	1.3617	1.3542	1.3477	1.3419	1.3367	1.3321	1.3280	1.3242	1.3208	1.3176
85	1.3555	1.3480	1.3413	1.3354	1.3302	1.3255	1.3213	1.3175	1.3140	1.3108
90	1.3500	1.3424	1.3357	1.3297	1.3244	1.3196	1.3153	1.3114	1.3079	1.3046
95	1.3451	1.3373	1.3306	1.3246	1.3191	1.3143	1.3100	1.3060	1.3024	1.2991
100	1.3407	1.3328	1.3259	1.3199	1.3146	1.3095	1.3051	1.3011	1.2975	1.2941
110	1.3329	1.3250	1.3179	1.3117	1.3062	1.3014	1.2967	1.2926	1.2888	1.2854
120	1.3265	1.3184	1.3112	1.3049	1.2993	1.2943	1.2898	1.2860	1.2816	1.2781
130	1.3210	1.3128	1.3055	1.2991	1.2934	1.2883	1.2837	1.2796	1.2760	1.2751
140	1.3163	1.3080	1.3006	1.2941	1.2883	1.2831	1.2784	1.2742	1.2704	1.2671
150	1.3122	1.3038	1.2964	1.2898	1.2839	1.2786	1.2738	1.2695	1.2656	1.2621
160	1.3086	1.3001	1.2926	1.2860	1.2800	1.2747	1.2698	1.2654	1.2614	1.2578
170	1.3054	1.2968	1.2893	1.2826	1.2766	1.2712	1.2663	1.2618	1.2578	1.2541
180	1.3026	1.2939	1.2863	1.2796	1.2735	1.2681	1.2631	1.2586	1.2545	1.2507
190	1.3000	1.2913	1.2837	1.2769	1.2708	1.2653	1.2603	1.2557	1.2516	1.2478
200	1.2977	1.2890	1.2813	1.2744	1.2683	1.2628	1.2577	1.2531	1.2489	1.2451
250	1.2890	1.2800	1.2721	1.2651	1.2588	1.2531	1.2479	1.2432	1.2388	1.2348
300	1.2831	1.2740	1.2660	1.2588	1.2524	1.2466	1.2413	1.2364	1.2320	1.2279
350	1.2788	1.2697	1.2615	1.2543	1.2478	1.2419	1.2365	1.2316	1.2271	1.2229
400	1.2755	1.2663	1.2581	1.2508	1.2443	1.2383	1.2329	1.2279	1.2233	1.2191
450	1.2728	1.2636	1.2554	1.2481	1.2415	1.2355	1.2300	1.2250	1.2204	1.2161
500	1.2704	1.2613	1.2531	1.2458	1.2391	1.2331	1.2277	1.2226	1.2180	1.2137
550	1.2682	1.2591	1.2510	1.2437	1.2371	1.2311	1.2256	1.2206	1.2159	1.2117
600	1.2660	1.2570	1.2490	1.2418	1.2352	1.2293	1.2238	1.2188	1.2141	1.2099
650	1.2638	1.2550	1.2471	1.2399	1.2334	1.2275	1.2221	1.2171	1.2125	1.2082

PHI-QUANTILES EPS=0.200

L/K	1	2	3	4	5	6	7	8	9	10
12	1.4794	1.5270	1.5362	1.5388	1.5397	1.5399	1.5399	1.5399	1.5397	1.5396
14	1.4483	1.4873	1.4921	1.4921	1.4911	1.4901	1.4891	1.4882	1.4874	1.4868
16	1.4257	1.4582	1.4596	1.4575	1.4551	1.4530	1.4512	1.4497	1.4484	1.4473
18	1.4085	1.4358	1.4346	1.4309	1.4273	1.4243	1.4218	1.4198	1.4181	1.4166
20	1.3949	1.4182	1.4148	1.4097	1.4052	1.4014	1.3984	1.3959	1.3938	1.3921
25	1.3710	1.3870	1.3796	1.3719	1.3655	1.3604	1.3562	1.3528	1.3500	1.3476
30	1.3554	1.3665	1.3565	1.3469	1.3392	1.3330	1.3280	1.3240	1.3206	1.3177
35	1.3444	1.3521	1.3400	1.3291	1.3204	1.3134	1.3078	1.3032	1.2994	1.2961
40	1.3362	1.3413	1.3278	1.3158	1.3063	1.2987	1.2926	1.2876	1.2834	1.2798
45	1.3300	1.3330	1.3183	1.3055	1.2953	1.2873	1.2807	1.2753	1.2708	1.2670
50	1.3250	1.3264	1.3107	1.2973	1.2866	1.2781	1.2712	1.2655	1.2607	1.2567
55	1.3209	1.3211	1.3046	1.2905	1.2794	1.2705	1.2634	1.2574	1.2524	1.2482
60	1.3176	1.3166	1.2995	1.2849	1.2734	1.2643	1.2568	1.2507	1.2455	1.2411
65	1.3147	1.3129	1.2951	1.2802	1.2684	1.2589	1.2513	1.2449	1.2396	1.2350
70	1.3123	1.3096	1.2914	1.2761	1.2640	1.2544	1.2465	1.2400	1.2345	1.2298
75	1.3102	1.3069	1.2882	1.2726	1.2602	1.2504	1.2424	1.2357	1.2301	1.2253
80	1.3083	1.3044	1.2854	1.2695	1.2570	1.2469	1.2387	1.2319	1.2262	1.2213
85	1.3067	1.3023	1.2829	1.2668	1.2540	1.2438	1.2355	1.2286	1.2228	1.2178
90	1.3052	1.3004	1.2808	1.2644	1.2515	1.2411	1.2327	1.2257	1.2197	1.2146
95	1.3038	1.2987	1.2788	1.2622	1.2491	1.2387	1.2301	1.2230	1.2170	1.2118
100	1.3024	1.2972	1.2770	1.2603	1.2471	1.2365	1.2278	1.2206	1.2145	1.2093
110	1.2998	1.2945	1.2740	1.2570	1.2435	1.2327	1.2238	1.2165	1.2102	1.2049
120	1.2970	1.2923	1.2715	1.2542	1.2405	1.2295	1.2205	1.2130	1.2066	1.2012
130	1.2939	1.2904	1.2693	1.2518	1.2379	1.2268	1.2177	1.2100	1.2036	1.1980
140	1.2904	1.2887	1.2675	1.2498	1.2358	1.2245	1.2152	1.2075	1.2010	1.1953
150	1.2862	1.2871	1.2659	1.2480	1.2339	1.2225	1.2131	1.2053	1.1987	1.1930
160	1.2814	1.2855	1.2644	1.2465	1.2322	1.2207	1.2113	1.2034	1.1967	1.1909
170	1.2760	1.2840	1.2631	1.2451	1.2307	1.2192	1.2097	1.2017	1.1949	1.1891
180	1.2697	1.2824	1.2619	1.2439	1.2294	1.2178	1.2082	1.2002	1.1934	1.1875
190	1.2627	1.2806	1.2607	1.2427	1.2283	1.2166	1.2069	1.1988	1.1920	1.1860
200	1.2550	1.2788	1.2596	1.2417	1.2272	1.2154	1.2057	1.1976	1.1907	1.1847
250	1.2040	1.2668	1.2534	1.2369	1.2228	1.2110	1.2012	1.1929	1.1858	1.1797
300	1.1298	1.2496	1.2452	1.2317	1.2187	1.2074	1.1978	1.1896	1.1824	1.1762
350	1.0179	1.2267	1.2344	1.2251	1.2141	1.2037	1.1946	1.1866	1.1797	1.1735
400	-1.0000	1.1983	1.2208	1.2169	1.2084	1.1995	1.1911	1.1837	1.1770	1.1711
450	-1.0000	1.1639	1.2044	1.2069	1.2015	1.1944	1.1871	1.1803	1.1741	1.1685
500	-1.0000	1.1223	1.1853	1.1952	1.1934	1.1884	1.1824	1.1765	1.1709	1.1657
550	-1.0000	1.0702	1.1635	1.1819	1.1842	1.1813	1.1771	1.1722	1.1673	1.1626
600	-1.0000	-1.0000	1.1385	1.1669	1.1738	1.1737	1.1710	1.1672	1.1632	1.1591
650	-1.0000	-1.0000	1.1098	1.1503	1.1623	1.1651	1.1642	1.1617	1.1586	1.1552

PHI-QUANTILES EPS=0.200

L/K	11	12	13	14	15	16	17	18	19	20
12	1.5395									
14	1.4862	1.4857	1.4853							
16	1.4464	1.4456	1.4449	1.4442	1.4437					
18	1.4154	1.4143	1.4134	1.4126	1.4118	1.4112	1.4106			
20	1.3905	1.3892	1.3881	1.3871	1.3862	1.3854	1.3847	1.3841	1.3835	
25	1.3455	1.3438	1.3422	1.3409	1.3397	1.3386	1.3376	1.3368	1.3360	1.3353
30	1.3152	1.3131	1.3112	1.3096	1.3082	1.3069	1.3057	1.3046	1.3037	1.3028
35	1.2933	1.2909	1.2888	1.2869	1.2853	1.2838	1.2825	1.2813	1.2802	1.2792
40	1.2767	1.2741	1.2718	1.2697	1.2679	1.2662	1.2648	1.2634	1.2622	1.2611
45	1.2637	1.2609	1.2584	1.2561	1.2542	1.2524	1.2508	1.2494	1.2481	1.2468
50	1.2532	1.2502	1.2475	1.2452	1.2431	1.2412	1.2395	1.2379	1.2365	1.2353
55	1.2446	1.2414	1.2386	1.2361	1.2339	1.2319	1.2301	1.2285	1.2270	1.2257
60	1.2373	1.2340	1.2311	1.2285	1.2262	1.2241	1.2222	1.2205	1.2190	1.2176
65	1.2311	1.2277	1.2247	1.2220	1.2196	1.2174	1.2155	1.2137	1.2121	1.2106
70	1.2258	1.2223	1.2191	1.2164	1.2139	1.2117	1.2097	1.2078	1.2062	1.2046
75	1.2211	1.2175	1.2143	1.2115	1.2089	1.2066	1.2046	1.2027	1.2010	1.1994
80	1.2171	1.2134	1.2101	1.2072	1.2046	1.2022	1.2001	1.1981	1.1964	1.1947
85	1.2135	1.2097	1.2063	1.2034	1.2007	1.1983	1.1961	1.1941	1.1923	1.1906
90	1.2102	1.2064	1.2030	1.1999	1.1973	1.1947	1.1925	1.1905	1.1886	1.1869
95	1.2073	1.2034	1.1999	1.1969	1.1941	1.1916	1.1893	1.1872	1.1853	1.1836
100	1.2047	1.2007	1.1972	1.1941	1.1913	1.1888	1.1864	1.1843	1.1824	1.1806
110	1.2002	1.1961	1.1925	1.1893	1.1864	1.1838	1.1814	1.1793	1.1772	1.1754
120	1.1964	1.1922	1.1885	1.1852	1.1822	1.1796	1.1771	1.1749	1.1730	1.1713
130	1.1932	1.1889	1.1851	1.1818	1.1787	1.1760	1.1735	1.1712	1.1692	1.1674
140	1.1904	1.1861	1.1822	1.1788	1.1757	1.1729	1.1704	1.1680	1.1659	1.1640
150	1.1880	1.1836	1.1797	1.1762	1.1731	1.1702	1.1676	1.1653	1.1631	1.1611
160	1.1859	1.1814	1.1775	1.1739	1.1708	1.1679	1.1652	1.1628	1.1606	1.1586
170	1.1840	1.1795	1.1755	1.1719	1.1687	1.1658	1.1631	1.1607	1.1584	1.1564
180	1.1823	1.1778	1.1738	1.1701	1.1669	1.1639	1.1612	1.1588	1.1565	1.1544
190	1.1808	1.1763	1.1722	1.1685	1.1652	1.1622	1.1595	1.1570	1.1547	1.1526
200	1.1795	1.1749	1.1708	1.1671	1.1638	1.1607	1.1580	1.1555	1.1531	1.1510
250	1.1743	1.1696	1.1653	1.1615	1.1581	1.1549	1.1521	1.1495	1.1470	1.1448
300	1.1708	1.1660	1.1616	1.1578	1.1542	1.1510	1.1481	1.1454	1.1429	1.1406
350	1.1681	1.1633	1.1589	1.1550	1.1514	1.1482	1.1452	1.1425	1.1399	1.1376
400	1.1657	1.1610	1.1567	1.1528	1.1492	1.1459	1.1429	1.1402	1.1376	1.1352
450	1.1634	1.1588	1.1546	1.1508	1.1472	1.1440	1.1410	1.1383	1.1357	1.1333
500	1.1609	1.1565	1.1525	1.1488	1.1454	1.1422	1.1393	1.1366	1.1340	1.1317
550	1.1582	1.1541	1.1503	1.1467	1.1435	1.1404	1.1376	1.1349	1.1324	1.1301
600	1.1551	1.1514	1.1479	1.1445	1.1414	1.1385	1.1358	1.1332	1.1308	1.1286
650	1.1518	1.1484	1.1452	1.1422	1.1393	1.1365	1.1339	1.1315	1.1292	1.1270



Kiadja a Központi Fizikai Kutató Intézet
Felelős kiadó: Gyimesi Zoltán
Példányszám: 20 Törzsszám: 86-05 /Utánnyomás/
Készült a KFKI sokszorosító üzemében
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